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REPORT NO. SP88-025

A TECHNICO-ECONOMIC EVALUATION OF CONVENTIONAL SYNTHETIC AND OXYGENATED GASOLINE BLENDING COMPONENTS

Final Report

by

J.G. Spiro, J.W. Engblom, H.F. MacEwen
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Work on this project was conducted under the auspices of
Canada Centre for Mineral and Energy Technology,
Energy, Mines and Resources Canada

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EXECUTIVE SUMMARY

At least since the early 1970s, the North American petroleum industry has been actively exploring new fuel formulations (and processing) for spark-ignition engines. "Cutting deeper into the barrel" - i.e. better utilization of residua and heavy fuel oils -, attempts to replace dwindling conventional crude reserves by energy sources such as heavy oil, tar sands, shale oil, natural gas, coal, and gradual elimination of lead antiknocks, have been the main driving forces. The objective of the present project was to consider the nature of Canadian "gasolines of the future" (early 21st century), their likely composition, properties and economics, the general business environment, and the state of art of octane and volatility correlations (with composition). The work involved literature studies on synthetic crudes and novel gasolines, preparation and characterization of fuel components and blends, economic evaluations. The latter employed a realistic refinery model (linear program), but must still be considered "rough cut", because of scant information on prices and the operating environment.

In terms of the resource base for "novel" spark ignition engine fuels, heavy oil/tar sands and natural gas deserve the most attention. There are no serious barriers to 25% synthetic crude in the crude slates of Canadian refineries - other than competition from cheap, imported crude oil. Propane and butane are potentially important raw materials for the production of oxygenated gasoline components (MTBE, cosolvents to be used with methanol) or for aromatization (BP-UOP Cyclar Process).

A number of conventional refinery stream samples (reformates, cat. cracked gasolines, alkylate, etc.), as well as a wide-range FCC gasoline from residuum cracking, were acquired for experimental studies. "Synthetic" reformates were prepared in a pilot plant unit from Syncrude naphthas. Detailed compositional analysis of these samples suggested relationships between chemical breakdown and performance. The samples were also used in gasoline blending experiments. The latter experiments have confirmed that the Ethyl Strategy Planner (ESP) computer program is suitable to estimate the blending octanes of hydrocarbon streams - whether conventional or "synthetic".

Much of the experimental work and most of the linear programming evaluations dealt with one of the promising oxygenated gasoline components: Oxinol 50 (50 volume % methanol-50 volume % tertiary butyl alcohol). Initial LP studies suggested gasoline compositions for assessing the performance of Oxinol 50, in terms of blending octanes and blending vapour pressure. Subsequently, the experimental data more or less confirmed volatility information available from the literature but Oxinol 50's efficacy as an octane appreciator was more difficult to quantify.

The fundamental conclusion of LP economic evaluations was that MTBE and Oxinol 50 both were economically attractive in a no-lead environment. The savings were only moderately sensitive to blending octanes and vapour pressures (within reasonable ranges).

SOMMAIRE-RECOMMANDATION

Depuis le début des années soixante-dix, l'industrie pétrolière nord-américaine étudie activement de nouveaux mélanges d'essence (et de nouveaux précédés de traitement) pour les moteurs à allumage par bougies. Les efforts en ce sens se sont concentrés principalement sur une meilleure utilisation des résidus et des mazouts lourds, sur le remplacement des réserves de brut classique (qui se font de plus en plus rares) par des sources d'énergie telles que le pétrole lourd, les sables bitumineux, les huiles de schiste, le gaz naturel et le charbon, ainsi que sur l'élimination graduelle des antidétonants à base de plomb. L'objectif du présent projet était d'étudier la nature des "essences de l'avenir" qui seront produites au Canada au début du 21e siècle, leur composition probable, leurs propriétés et leurs coûts de fabrication; on s'est également penché sur le climat économique général et l'état des connaissances en matière de corrélation entre l'indice d'octane et la volatilité et la composition des mélanges. Les travaux consistaient à faire une revue de la littérature traitant des bruts synthétiques et des essences nouvelles, à préparer et à décrire les constituants des essences de même que les mélanges eux-mêmes, et à effectuer des évaluations économiques. Pour ces dernières, on s'est servi d'un modèle réaliste de raffinerie (programmation linéaire). Ces évaluations doivent toutefois être considérées comme approximatives en raison de l'insuffisance de données sur les prix et les conditions d'exploitation.

Les ressources les plus prometteuses pour la production de carburants nouveaux pour les moteurs à allumage par bougies sont le pétrole lourd, les sables bitumineux et le gaz naturel. Il n'existe aucun obstacle majeur à l'utilisation par les raffineries

canadiennes de diètes de brut comprenant 25% de brut synthétique -- si l'on exclut la concurrence avec le brut importé à bas prix. Le propane et le butane pourraient devenir des matières premières importantes pour la production de constituants d'essence oxygénés (EBTM et cosolvants utilisés avec le méthanol) ou pour l'aromatisation (procédé Cyclar BP-UOP).

Un certain nombre d'échantillons de produits de raffinage classiques (reformats, essences de craquage catalytique, alkylat, etc.) de même qu'une essence de CCF à intervalle de distillation étendu et obtenue par craquage de résidus, ont servi à des études expérimentales. Des reformats "synthétiques" ont été préparés dans une usine pilote à partir de naphtas de brut synthétique. Des analyses détaillées de ces échantillons ont indiqué qu'il pourrait y avoir un lien entre la composition chimique et le rendement. Les échantillons ont également servi à des expériences portant sur les mélanges d'essence. Ces expériences ont confirmé que le logiciel ESP (Ethyl Strategy Planner) permet d'évaluer convenablement l'indice d'octane des mélanges d'hydrocarbures, tant classiques que synthétiques.

Une grande part des expériences et la majeure partie des évaluations en programmation linéaire ont porté sur un des constituants d'essence oxygénés prometteurs, l'Oxinol 50 (50% en volume de méthanol et 50% en volume de butanol tertiaire). Des études initiales en programmation linéaire ont suggéré des compositions permettant d'évaluer le rendement de l'Oxinol 50 en ce qui à trait à l'indice d'octane et à la tension de vapeur. Les résultats des expériences menées ultérieurement ont plus ou moins confirmé les données sur la volatilité dont la littérature faisait état, mais l'efficacité de l'Oxinol 50 comme antidétonant était plus difficile à mesurer.

La principale conclusion qu'on peut tirer des évaluations en programmation linéaire est que l'EBTM et l'Oxinol 50 offrent tous deux des possibilités intéressantes d'un point de vue économique comme substituts aux antidétonants à base de plomb. Les variations d'indice d'octane et de tension de vapeur n'ont qu'une incidence modérée sur les économies réalisées (à condition que les écarts ne soient pas trop grands).

ABSTRACT

This project has dealt with the examination of certain technical aspects (primarily the composition, knock resistance and volatility characteristics) and the economics of Canadian "gasolines of the future" (to be marketed, say, in the year 2,000).

In terms of the resource base for "novel" spark ignition engine fuels, heavy oil/tar sands and natural gas deserve the most attention. There are no serious barriers to 25% synthetic crude in the crude slates of Canadian refineries - other than competition from cheap, imported crude oil. Propane and butane are potentially important raw materials for the production of oxygenated gasoline components (MTBE, cosolvents to be used with methanol) or for aromatization (BP-UOP Cyclar Process).

A number of conventional refinery stream samples (reformates, cat. cracked gasolines, alkylate, etc.), as well as a wide-range FCC gasoline from residuum cracking, were acquired for experimental studies. "Synthetic" reformates were prepared in a pilot plant unit from Syncrude naphthas. Detailed compositional analysis of these samples suggested relationships between chemical breakdown and performance. The samples were also used in gasoline blending experiments. The latter experiments have confirmed that the Ethyl Strategy Planner (ESP) computer program is suitable to estimate the blending octanes of hydrocarbon streams - whether conventional or "synthetic".

Much of the experimental work and most of the linear programming evaluations dealt with one of the promising oxygenated gasoline components: Oxinol 50 (50 volume % methanol-50 volume % tertiary butyl alcohol). Initial LP studies suggested gasoline compositions for assessing the performance of Oxinol 50, in terms of blending octanes and blending vapour pressure. Subsequently, the experimental data more or less confirmed volatility information available from the literature but Oxinol 50's efficacy as an octane appreciator was more difficult to quantify.

The fundamental conclusion of LP economic evaluations was that MTBE and Oxinol 50 both were economically attractive in a no-lead environment. The savings were only moderately sensitive to blending octanes and vapour pressures (within reasonable ranges). Even when the unit price of Oxinol 50 was raised from 25¢/L to 33¢/L (approximately), it still offered some economic benefits.

1. INTRODUCTION

The overall objective of the present project has been to examine certain technical aspects (primarily the composition, knock resistance and volatility characteristics) and the economics of Canadian "gasolines of the future" (to be marketed, say, at the end of this century).

At least since the early 1970s, the petroleum industry has been actively exploring new fuel formulations and processing for spark-ignition engines. There have been three main driving forces behind this search: (i) Better utilization of crude oils by "cutting deeper into the barrel", i.e., upgrading residua. Declining demand for heavy fuel oils has accelerated this trend; (ii) Attempts to replace dwindling conventional crude reserves by energy sources such as heavy oil, tar sands, shale oil, natural gas and coal; and (iii) Gradual elimination of lead antiknocks, creating a demand for higher octane streams.

Canada, like other countries, is faced with a steady decline in crude oil supply from conventional sources. However, light oil production from frontier areas and the almost limitless Canadian reserves of heavy oil and tar sands could replace conventional oil. Even if international crude oil prices will remain low, the upgrading of heavy oil/bitumen will be commercially important in Canada. The latter facet of gasoline technology will, therefore, be discussed here in some detail.

Lead "phase-down" may have a more revolutionary influence on spark-ignition engine fuels than "synthetic" crude oils; namely, it could lead to widespread penetration of the markets by alcohols and ethers. This aspect of gasoline technology also deserves a more thorough discussion.

There is much in common between the technologies of upgrading conventional residua, heavy oils and bitumen. For all three, it is customary to classify various processes into carbon rejection and hydrogen addition technologies, although generally both types of processing are required (one following the other) to produce transportation fuels. Among carbon rejection technologies, Delayed Coking (Suncor), Fluid Coking (Syncrude) and Flexicoking, an extension of the Fluid Coking process [1], are commercially

proven, and several others are promising (Eureka process [2], asphalt residual treating [ART, Reference 3], metal resistant cat. cracking catalysts, Taciuk direct retorting of oil sands). The best known and commercially proven hydrogenation technologies are H-Oil, LC-Fining and Gulf HDS, with various options available as to degree of conversion and catalysts. Here again, new concepts are being explored, such as slurry reactor processes using inexpensive, once-through (throw-away) additives in thermal hydrocracking (e.g. CANMET, VEBA-Combi-Cracking, UOP Aurabon) and donor solvent processes that represent milder hydrotreating (e.g. Gulf DRB).

The number of combinations and permutations of heavy oil upgrading processes seems endless. For instance, partial upgrading at the production site (cracking, visbreaking, deasphalting) may be followed by more thorough processing at refineries - or, at the other extreme, it could be desirable to combine upgraders with refineries, manufacturing finished products close to the resource's location [4]. Process selection is a multi-faceted task [5], and "changing perceptions of risk and improved price/cost relationships could result in more upgrading capacity" [6].

It is easier to draw a picture in terms of the chemistry of the gasolines that will be produced than to predict which specific processes will be the most successful or most widely employed. Hydrocarbon fuels boiling in the gasoline range will be made up of much the same molecules as contained in present-day straight run naphthas, isomerates, reformates, cat. cracked gasolines, alkylates and polymerization gasolines. Differences between, say, a conventional and "synthetic" reformate, or between a conventional FCC gasoline and one from residuum cracking, are not expected to be revolutionary*, and will probably be adequately represented by samples obtained in the present project. However, in recent years, alcohols and ethers have begun to acquire importance as

*This does not mean that the differences are insignificant. One of the less obvious compositional effects is the relatively high mono-aromatics content of gas oils derived from heavy oil/bitumen upgrading; this will lead to better octane quality cat. cracked gasolines.

motor fuel components, even in North America. The prospects of these "oxygenates" are somewhat controversial and may be summarized as follows:

Although ethanol has been a popular gasoline extender in Latin America for many years, in Canada and the United States it either has not been able to gain strength or has been very dependent on tax "breaks" [7]. Large fermentation plants and major gasohol (10% ethanol in gasoline) production still do not appear to be economical in Canada. However, most recently, the State of Colorado has announced rules that will make the use of oxygenated fuels mandatory in Denver and some other cities, during the winter months [8], the aim being to combat carbon monoxide emissions. "The prospect of other states and Canada following suit to reduce lead and carbon monoxide emissions has two Alberta-based companies preparing blueprints for major fuel-alcohol plants that would use western Canadian grains and sugar beets to provide the gasoline additive" [9]. On the whole, though, methanol/cosolvent systems and methyl-tertiary butyl ether (MTBE) are more likely to be used as octane improvers in Canada.

Methanol-gasoline blends are currently not being marketed in the United States but their technology, especially with tertiary butyl alcohol as the cosolvent [10], is quite well established. Some concerns remain about materials/fuel compatibility and quality of the delivered product [11], but the most difficult questions relate to economics.

First of all, the role of methanol ties in with the broader subject of converting natural gas to fuels. At this time, synthesis gas offers the best route to methanol [12], and it seems clear that coal cannot compete with natural gas as the basic feedstock [13]. Once methanol is produced for motor fuel applications, it may be preferable, however, to convert it to gasoline, e.g. via the Mobil MTG process. This is the approach that was elected by the New Zealand government. Synthesis gas is not cheap though, and the natural gas-acetylene-ethylene-gasoline route [14], using the Mobil olefin oligomerization process as its final step, appears to be more attractive economically. Taking all the possibilities into consideration, it is not clear whether in the long run methanol will be able to compete as a gasoline component.

Methyl-tertiary butyl ether (MTBE) is another important oxygenate - and one that is less controversial than alcohols from the technical standpoint, because it is more hydrocarbon-like. The primary problem facing MTBE producers is a shortage of raw material isobutylene. Adequate butane supplies from both refinery and natural gas sources suggest that processes such as CATOFIN dehydrogenation of isobutane, followed by etherification with methanol [15] will be an economical source of MTBE. Currently, considerable attention is being paid to restricting gasoline volatility [8], and this could also be an important boost for MTBE, making more butane available as oxygenate feedstock and increasing the need for high-octane blending components. Similar comments apply to the synthesis of isopropanol and butanols - the most promising cosolvents that can be used with methanol.

In examining the likely sources of Canadian gasolines at the end of this century, a few more trends must be considered:

(i) It is generally thought that international crude oil prices will remain stable or even decline over the next few years. It is, therefore, unlikely that expensive coal liquefaction projects - with or without synthesis gas as the intermediate product - will generate appreciable volumes of automotive fuels in Canada before the 21st century.

(ii) Shale oil is potentially a very important resource in North America. It is usually thought of as a feedstock to produce (primarily) turbine and diesel fuels, but it is possible to obtain 100+ vol.% gasoline based on raw shale oil [16]. In the United States, oil shales have received considerable attention - on and off - but in Canada they are frequently ignored as an energy resource. Alternatively, shale oil is considered here strictly as a raw fuel [17], retorting and further refining not being planned. On balance, it seems unlikely that it will be a significant factor in Canadian gasoline production over the next 15 years.

(iii) New ideas in gasoline processing - for instance the BP-UOP Cyclar Process, which aromatizes propane and butanes [18] - could have a major impact, equally important as political and economic developments.

In summary, while there are many technical and economic uncertainties, it is likely that "synthetic" hydrocarbons* and oxygenates will play significant roles in Canadian gasolines at the end of this century. Many future developments are difficult or impossible to predict, but some important technical details can be clarified now. Specifically, it has been possible to formulate some "gasolines of the future", investigate their composition and consider how it will affect performance, determine octane and volatility blending values experimentally, and conduct economic evaluations taking cognizance of the manifold constraints that govern "real-life" refinery operations. The sections that follow will report the work accomplished and its implications.

2. OVERVIEW OF THE INVESTIGATIONS

The contract loosely specified the hydrocarbon streams to be characterized in the experimental studies, and it gave a list of oxygenated fuel components. Some details were left open, pending the outcome of preliminary studies. It turned out that potential suppliers were unwilling to provide naphthas from upgrading processes (CANMET, H-Oil, LC-Fining), or insisted on secrecy agreements that were unacceptable. Accordingly, more reliance had to be placed on preparing "synthetic" streams in the pilot plant. The number of oxygenates to evaluate was greatly reduced, in order to avoid excessive overlap with the "Investigation of Process Conditions for the Synthesis of Liquid Distillates from Light Olefins and Methanol" contract**. The final list of samples, and details of the selection process, will be discussed in Section 3.

The preparation of "synthetic" reformates was conducted in a Petro-Canada Products R&D Centre hydrotreating and reforming pilot

*In the present report, "synthetic" gasoline components are defined as streams that are produced from feedstocks other than conventional crude oil, such as natural gas, heavy oil, bitumen or residua. There is some overlap, but alkylates, isomerates, polymerization gasolines - products well established in conventional petroleum refineries - will not be regarded as synthetics here.

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plant. Syncrude naphthas are often considered difficult to reform [19], but the pilot plant yields were satisfactory. Particulars of this work are given in Section 4.

All hydrocarbon samples were inspected in accordance with accepted practices, and were also analyzed by mass spectrometry and high-resolution gas chromatography. These detailed analyses have provided opportunities to correlate chemical composition with gasoline properties and processing, as discussed in Section 6. The analytical methodology is described in Section 5.

The starting point for economic evaluations was an existing Petro-Canada refinery Linear Program (LP) model. Some modifications were made to minimize operating constraints specific to this particular refinery. Current lead levels were employed in the initial work, but only manganese additive (MMT*) was allowed in the "Year 2000" scenario. Present-day gasoline specifications were to be achieved at the end of this century with increased quantities of Syncrude feed, and if economical, with methanol-cosolvent or MTBE octane improver. Technological improvements, such as cat. cracking catalysts yielding higher octane gasolines, were also taken into consideration. The basic assumptions of LP evaluations will be elaborated further in Section 7.

Some more specific assumptions involved crude, hydrocarbon stream and oxygenate prices, blending octanes, vapour pressure and water miscibility of oxygenated gasolines (Section 8). The initial calculations were based on literature data or the existing Petro-Canada data base, but even for hydrocarbon fuels the octane blending behaviour was studied experimentally as well (Section 8.1). It was confirmed that Ethyl Corporation's Ethyl Strategy Planner (ESP) computer program [20] predicted blending non-linearities well for hydrocarbons. No such aids were available for gasolines containing alcohols. Indeed, the experimental data suggested (Section 8.2) that there was at least a 10-15 octane number uncertainty in methanol-tertiary butyl alcohol blending values. The significance of this was explored via LP sensitivity studies.

*Methylcyclopentadienyl Manganese Tricarbonyl

Results of the Linear Programming evaluations are discussed in detail in Section 9. Sensitivity studies have pointed out some uncertainties, but on the whole, the outlook for oxygenates in "gasolines of the future" is good. Even a 15 octane number difference in blending values seems less important than broad economic, political and environmental developments that have been considered or alluded to in the Introduction. The fact that the LP work utilized a model (albeit modified) of an existing refinery, increases the realism of the results.

The overall conclusions reached are the subject of Section 10.

3. FINALIZATION OF THE LIST OF GASOLINE COMPONENTS FOR EXPERIMENTAL STUDIES

The original list of hydrocarbon stream samples specified in the contract was as follows:

- Butane(s)
- Light Straight Run Gasoline (Deisohexanizer Overheads)
- Four different conventional reformates
- Two light and two heavy reformates containing high proportions of "synthetics"
- Three different conventional cat. cracked gasolines
- Light and heavy cat. cracked naphthas (one of each) from residuum processing
- Alkylate
- Polymerization Gasoline
- Udex Raffinate

The above represented a sufficient variety of refinery streams to provide a good basis for experimental investigations. The emphasis on reformates reflected the considerable differences shown by commercial reformates with respect to boiling range and octane number, as well as the importance of high-severity reforming in replacing octane-barrels lost to lead phase-down. The chemical composition of cat. cracked gasolines is more complex than that of reformates; here, crude source and especially boiling range are important parameters. Wide-range FCC naphthas can be

split into light, medium and heavy cuts. This improves blending flexibility, because usually the middle cut has the lowest octane [21].

Most of the "conventional" gasoline component samples were obtained from Petro-Canada's Port Moody Refinery. The crude slate there (at the time of furnishing the samples) was a mix of Peace River and Texaco Light (western Canadian conventional crudes) with 25% syncrude, based on Athabasca bitumen. Polymerization gasoline and Udex raffinate were acquired from Gulf Canada's Montreal East Refinery, at the end of 1985. The butane used in gasoline blending experiments was C.P. grade butane from Matheson (minimum 99.0 wt.% normal butane).

"Synthetic" reformates were prepared in the pilot plant. The feedstocks for this work were synthetic crude from Syncrude Co. Ltd. (fractionated at Sheridan Park to obtain a 130-200°C boiling range heavy naphtha), and a Syncrude naphtha* from the former Gulf Canada (now Petro-Canada) refinery at Edmonton. (The latter, too, was fractionated at the Petro-Canada Products R&D Centre, to obtain a 70-130°C boiling range light naphtha.) Reforming to different severities yielded the four fuel components specified in the contract; details of the pilot plant work are provided in Section 4.

Fractionation of a wide-range Port Moody cat. cracked gasoline yielded the three "conventional" FCC naphthas, and similar treatment of another cat. cracked gasoline, from Murphy Oil's Meraux, Louisiana refinery, led to the samples from residuum cracking**.

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*Naphthas from other upgrading processes could not be obtained.

**Murphy Oil's feed was a mixture of 60-70% residuum with 30-40% gas oil, cracked via UOP Inc.'s RCC (Residual Catalytic Cracking, see Reference 22) Process.

The foregoing selection of conventional and "synthetic" gasoline components was approved by Dr. H. Sawatzky (Scientific Authority). Samples of nine oxygenates (methanol, ethanol, isopropanol, n-butanol, isobutanol, tert. butyl alcohol, methyl tert. butyl ether, amyl methyl ether, di-isopropyl ether) were also ordered at the time. At the April 10, 1987 project review in Ottawa [23] it was decided, however, that there was excessive overlap with the "Investigation of Process Conditions for the Synthesis of Liquid Distillates from Light Olefins and Methanol" contract (DSS File 06SQ.23440-5-9113), so that final gasoline blending experiments under the present project would be limited to mixtures with Oxinol 50 (50 volume % methanol - 50 volume % tertiary butyl alcohol) as the oxygenated component. (This decision was in accordance with the present contract's stipulation: "Related work is being carried out in another contract and any work here shall be complementary.")

4. PREPARATION OF "SYNTHETIC" REFORMATES

Two different crude samples were used in preparing the Syncrude reformates (see Section 3). The light naphtha contained approximately 10 ppm by weight of sulfur, sufficiently low to allow reforming without pre-treatment in the pilot plant (but not in a refinery!). A Pt/Re bimetallic catalyst was employed, at 1.5 hr^{-1} LHSV and 2.34 MPa (340 psia). To obtain nominal 90 and 95 RON (clear) reformates, the average catalyst bed temperatures required were estimated at 460 and 474°C, respectively. The actual octane numbers and API gravities of the products obtained are given in Table 4.1, whereas Table 4.2 (computer generated) shows the material balances achieved.

The heavy naphtha had a sulfur content of 300 ppm; mild hydrotreatment was necessary to reduce it. (Normally, bimetallic reforming catalysts require feed sulfur levels of 0.5 ppm by weight or less.) Katalco NM-506 catalyst was used, at 335°C, 3.45 MPa (500 psia) and 1.5 hr^{-1} LHSV. These conditions were mild enough that little or no saturation took place and the density only changed from 0.8035 to 0.8016 g/mL. The collected product was caustic washed to remove trace H_2S and was dried on mole sieve to remove residual water. The RON of this reformer feed was 65 (value determined in a blend).

Heavy naphtha reforming was conducted at 1.5 hr^{-1} LHSV, 2.34 MPa (340 psia) and temperatures of 483 and 500°C, to produce final products with research octane numbers of 97 and 102.8, respectively. Due to the limited quantity of feed, these final products were augmented by combining them with line-out product, which had lower octane value. As a result the octane numbers were reduced to 92 and 98.8 respectively. In order to determine an approximate unit yield, a yield curve was generated based on the material balance for each run. The material balances are given in Table 4.3 and the yield curve is shown in Figure 4.1. The lower octane numbers of the product blends were used with this curve to project the unit yield corresponding to the new octane values. Figure 4.1 shows the interpolated values of 77.4 wt.% yield for 98.8 RON and 83.4 wt.% yield for 92 RON.

The yield of the higher octane product was below the minimum target, but this was probably due to the pilot plant being an isothermal reactor (vs. the adiabatic commercial reactors).

Inspections and analyses of all four Syncrude reformates are given in Section 6, where the similarities and differences between these and conventional reformates are also discussed.

5. ANALYTICAL METHODOLOGY

5.1 Gas Chromatographic Detailed Component Analysis

The gas chromatographic component analyses were performed on an Hewlett-Packard "PNA/PONA Analyzer". This consisted of an HP5880A capillary gas chromatograph equipped with a fused silica column (50 m x 0.20 mm), having a 0.52 μm film of cross-linked methyl silicone. In some cases, the C_4/C_5 component concentrations were confirmed, using a packed column (squalane/bis(2-ethoxyethyl) adipate). The capillary GC analytical results are reported in two sets of tables, one set giving individual hydrocarbon concentrations, the other listing them according to carbon number and group type.

5.2 Mass Spectrometric Detailed Compositional Analysis

Non-olefinic samples were analyzed on a CEC 21-103C mass spectrometer, by an in-house calibrated (modified) ASTM D2789 method. Olefinic samples were handled by a low-eV method developed in-house.

5.3 Summary of Analytical Data (Combined GC and MS Data)

In the summary tables, GC data were utilized for C_4-C_8 saturate components in non-olefinic samples and for C_4-C_6 saturates in olefinic samples; mass spectrometric data were accepted for all other compounds, with appropriate normalizations.

5.4 Gas Chromatographic Boiling-Range Distribution Analysis

The reported GC simulated distillation analyses were performed on an HP5880A gas chromatograph. The data were processed on a P-E3410 lab computer, using an in-house program.

6. INSPECTIONS AND ANALYSES OF HYDROCARBON STREAM SAMPLES; IMPLICATIONS

Inpsections of the "conventional" gasoline component samples are given in Table 6.1. Tables 6.2 and 6.3, respectively, show the results of the standard tests on Syncrude reformates and cat. cracked gasolines from residuum cracking. Two anomalous properties of the "novel" fuels ought to be pointed out: (a) the heart cut (80-140°C) of the Murphy Oil cat. cracked gasoline has higher RON than the 140°C+ bottoms; and (b) the Syncrude heavy reformates have very high (approximately 260°C) end points. These anomalies can be related to process chemistry if one refers to the detailed compositional analyses of Tables 6.4 and 6.5.

It is often assumed [24] that feed and product aromatics contents are the most important determinants of octane number, and that they are also responsible for the increasing octane number of FCC gasoline cuts with boiling point (after an initial decline). The analytical data indicate that - at least sometimes - this is an oversimplification. For the Murphy Oil sample representing residuum cracking, the rapid decrease in olefin and cyclo-olefin contents at high boiling points (more pronounced than for the

conventional FCCG ex Port Moody) has a larger effect than the increased aromatics content, resulting in an unusual octane-boiling point relationship (Table 6.5). This has significant practical consequences: the usual procedure [21] of isolating a lower-octane middle cut for improved blending flexibility is vitiated. The anomaly may be caused by the "exceptional cracking capability" of some catalysts used in residuum processing [25] and may require some attention by catalyst manufacturers. We understand, however, that even though the octane number of heavy cat. cracked gasolines is difficult to predict, the anomaly we have observed is not typical of residuum cracking [26], nor is the increased MON when RON is already declining.

For the sake of completeness, compositional analyses have also been carried out on a Trafalgar wide-range FCC gasoline, used in blending experiments. Results of the latter characterizations are given in Appendix I.

Table 6.4 contains appreciable information relating to reformate chemistry. The heavy ends of Syncrude reformates are seen to be C_{10}+ aromatics, and their low volatility suggests multi-substituted benzene derivatives. The latter kind of structure appears to be prevalent in synthetic middle distillates as well [19]. There is also some suggestion that conventional reformates are more paraffinic than their synthetic counterparts. Still, the differences between Port Moody (25% synthetic) and Syncrude (100% synthetic) heavy reformates are not striking, and are obscured by the lack of detailed gas chromatographic analyses at carbon numbers above C_8. It is easier to draw definite conclusions from the comparison of Port Moody and Syncrude light reformates, as follows.

Port Moody sample D85-116 and Syncrude reformate 86-P12-022 had similar octane numbers (although the "synthetic" gasoline exhibited much higher sensitivity*, no doubt because of its higher cyclic hydrocarbon content), as well as similar boiling ranges. It was a simple matter to isolate from the gas chromatographic analyses overlapping fractions boiling between 80°C and 144°C at atmospheric pressure (benzene to o-xylene); these represented

*Sensitivity = Research octane number minus Motor octane number of a gasoline.

approximately 75% of the Port Moody and 80% of the Syncrude reformate (Tables 6.7 and 6.8). Table 6.9 shows the remarkable similarity of these two reformate fractions in terms of the individual chemical concentrations. Clearly, whereas the processing conditions required to reform synthetic naphthas may be different from those needed for conventional feedstocks, light reformate product quality will often be indistinguishable for the two. This agrees with our experience (Section 8.1) that Ethyl Corporation's ESP computer program [20] "handles" synthetic reformates very well.

Since reforming is currently the most important octane upgrading technology, it is of interest to examine briefly some approaches to process optimization. Comparison of the compositions of Port Moody Prefractionator Overhead (P.O.H., a straight-run gasoline) and Montreal Udex Raffinate (the naphtha left behind after aromatics extraction from a light reformate) provides this opportunity. As with the conventional and Syncrude reformates, this meant examining identical boiling range portions of the two samples; in this case, hydrocarbons boiling between 60°C (2-methylpentane) and 111°C (toluene) at atmospheric pressure.

Udex Raffinate is a stream that was processed through a reformer and then the aromatics were extracted. Theoretically, it contains neither aromatics nor aromatics precursors. Measured against this "standard", we note significant excess concentrations of methylcyclopentane, benzene, cyclohexane and other cycloparaffins in P.O.H. We are paying this price for saving on reforming costs and for inefficient fractionation - there may be room for improvements. However, it was outside the scope of the present project to conduct an actual optimization study.

Results of the mass spectrometric and gas chromatographic analyses of Port Moody Prefractionator Overhead and Montreal Udex Raffinate have been compiled into the same format as the cat. cracked gasoline and reformate analyses. Together with the Port Moody C_4 Alkylate and Montreal Polymerization Gasoline analyses, they are shown in Table 6.6. This completes the analytical data on fuel components.

7. BASIC ASSUMPTIONS OF THE ECONOMIC EVALUATIONS

As was mentioned in the Overview, economic evaluations employed an existing Petro-Canada refinery Linear Program (LP), with appropriate modifications. Such programs incorporate the manifold constraints that govern refinery operations, hence their output reflects reality. On the other hand, some operating restrictions can be highly specific to a given refinery and may lead to a biased assessment of, say, the value of oxygenates as octane improvers. Constraints of the latter type were minimized.

Major types of information characterizing refinery operations, embodied in linear programs, are:

(i) unit yields and capacities, including yield models which relate product flow rates and quality to feed quality and operating conditions
(ii) crude and product slates
(iii) product quality specifications
(iv) costs such as crude, raw materials (including oxygenates), catalyst and antiknock purchases
(v) product values (sales)
(vi) tankage and other operating restrictions
(vii) inventories

Using the above data - linked together by "linear constraints", e.g. between gasoline composition and octane number - the LP selects a combination of "activities" that minimize the total operating costs. In terms of the studies conducted under the present contract, the main outputs of the LP were gasoline blending "recipes", information as to <u>how</u> cost savings were accomplished, as well as their size. (Smaller excesses of low-octane light gasoline, reduced antiknock and reforming costs are some of the items particularly worth mentioning.) Formulation and implementation of the LP utilized the Generalized Refining - Transportation - Marketing Planning System licensed by HAVERLY SYSTEMS, INC., Denville, New Jersey.

A number of broad assumptions relating especially to gasoline production were incorporated into the LP model:

7.1 Current specifications to be maintained, but no lead allowed in the year 2000.

7.2 Apart from lead removal, no other changes in gasoline quality specifications over the years.

7.3 Manganese additive (MMT) allowable throughout, up to a maximum level of 0.06 g MMT/U.S. gallon fuel.

7.4 Total product demands placed on the refinery were to give a crude charge at least 80% of listed capacity.

7.5 The gasoline to distillate ratio was set at 1.25, to reflect the current Canadian national average.

7.6 Shifts in the gasoline/distillate demand ratio were to be accommodated by "importing" diesel fuel (if necessary) from a refinery with excess capacity.

7.7 In the Year 2000 scenario (no leaded gasoline demands), unleaded gasoline requirements were defined at 20% super - 80% regular.

7.8 C_5/C_6 stream sales were allowed, to remove LP infeasibilities.

7.9 Basic octane improvement schemes for the year 2000 were: higher octane cat. cracked gasolines (to reflect improved catalysts), full conversion of light olefins to alkylate or polymerization gasoline, higher severity reforming.

7.10 The price of syncrude was reduced relative to conventional crude, to reflect expected changes by the end of the century. However, syncrude was limited to 25 volume % in refinery feedstock, to avoid complications relating to Diesel quality.

The above ground rules and assumptions set the basic scenarios; but there were still many details to be considered, such as oxygenate prices and blending values. These will be discussed in Section 8, including the experimental confirmation (or otherwise) of certain mixture properties.

8. PRICES, BLENDING VALUES, WATER TOLERANCE

8.1 Input Data Relating to Hydrocarbon Streams and Confirmation of Blending Octanes

The main thrust of the economic evaluations was assessment of the prospects of oxygenates in Canadian gasolines. In addition, however, the price of synthetic crudes was lowered compared to conventional crudes even in the base case for the year 2000 (no oxygenates), to reflect the anticipated, increased availability of the former.

To keep the simulations simple, Peace River and Peace River-Syncrude Blend constituted the entire crude slate of the refinery. These were appropriate feed choices for a Western Canadian refinery and allowed a realistic study of the conventional versus synthetic crude circumstances.

Peace River-Syncrude pipeline blend typically contains 25% synthetic crude. The LP was allowed to "purchase" only the blend, not pure Syncrude; this placed a limit on the utilization of synthetic crude, as it has been mentioned in Section 7.

Syncrude price reduction was modest. In the original LP data base Peace River Crude had been priced at $37.36/bbl, Peace River-Syncrude Blend at $37.25/bbl; the latter price was reduced to $36.93/bbl. (I.e., the price of 100% Syncrude was assigned to the blend.) This reduction was so effective that during the January-March and April-June Quarters the LP "purchased" almost exclusively Peace River-Syncrude Blend, and even over the entire year, 70 vol.% of the total crude purchases was the mixture and only 30 vol.% was straight Peace River Crude in the year 2000 base case.

A certain synergism was detected between the utilization of Syncrude and oxygenates. Generally, when the gasoline formulations included MTBE or alcohols, the LP elected to purchase 95+ vol.% Peace River-Syncrude Blend and less than 5 vol.% Peace River Crude over a year.

Pricing of the C_5/C_6 naphtha stream was also important: it had a major effect on oxygenate economics. The reduction of C_5/C_6 stream sales (in effect, substituting light straight run gasoline for crude) was the most important driving force towards cost savings with oxygenates. The lower the value of light, paraffinic gasoline, the more attractive will oxygenates be. If low-octane naphtha can be routed to steam crackers as feedstock, the octane shortage will be alleviated. Isomerization to a higher-octane C_5/C_6 stream is also an attractive possibility - but if the capacity is lacking, excess light gasoline can become a liability rather than an asset. The complexities of this matter have not been thoroughly reviewed in the present project, but a C_5/C_6 naphtha unit price of $25.00/bbl (15.72¢/L) seemed reasonable and was used in the economic evaluations. As a matter of fact, a C_5/C_6 light gasoline/crude price ratio very similar to the one discussed here has been employed in a recent Petro-Canada study of East Coast crudes.

As is frequently found with unleaded gasolines, manganese additive was economical both in hydrocarbon fuels and in oxygenated blends. The price of this additive, used in our LP evaluations, was 6.88¢/g MMT. Crude, C_5/C_6 stream and MMT prices are included in Table 8.3, which contains cost information on oxygenates too, as input into the LP.

The contract also called for an appraisal of the blending octanes of hydrocarbon streams. (Were the values in the initial LP data base realistic? Even if they were, was there evidence that different correlations would be required for "synthetic" fuel components?) This was conducted experimentally and by means of computer simulations, as follows.

First, it was established that for eight different regular unleaded gasolines, which had been formulated without manganese antiknock and had actually been produced at Petro-Canada's Port Moody Refinery, there was good agreement between measured RON and MON values, knock ratings calculated from blending octane numbers in the initial LP data base, and octane numbers calculated with the Ethyl Strategy Planner (ESP) computer program [20]. A brief description of Ethyl Corporation's predictive techniques is given in Appendix II; input data into the latter program were component properties measured at Sheridan Park (Section 6). The LP and ESP appeared to be suitable tools to deal with conventional gasolines; what remained to be explored was their performance with "synthetic" and other unusual components.

Broad plans for the experimental program were agreed upon at a review meeting, held in Ottawa, on January 21, 1986. The blend design involved five base gasolines, out of which three: summer and winter grade premium unleaded and a regular unleaded fuel were suggested by LP runs. The fourth (regular unleaded) formulation represented recent refinery production, and the fifth (regular unleaded) gasoline corresponded to "forcing" low-octane light reformate into the unleaded pool. Conventional and residuum-based cat. cracked gasoline fractions, light and heavy Syncrude reformates, Udex raffinate and polymerization gasoline were then substituted for the "standard" streams, mostly one at a time. The detailed blend compositions, approved by Dr. H. Sawatzky (scientific authority) on February 27, 1986, are shown in Table 8.1.

The 18 gasolines of Table 8.1 were then prepared and knock rated. Experimental Research and Motor Octane Numbers, together with ratings predicted* by ESP, are given in Table 8.2.

The differences between measured and predicted Research Octane Numbers were small and apparently normally distributed, with a mean of approximately -0.25 and a standard deviation of 0.23. This model suggests that ESP can be relied upon without adjustment to predict the RON change when one component is substituted for another. Indeed, the mean error of the latter type of calculation was only 0.1 for the 13 substitution blends of Table 1, with a standard deviation of 0.24. Clearly, ESP handles well the less conventional components. (The predicted Research Octane Numbers show the same bias (-0.28) for base gasolines as for the substitution blends.)

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*The required input data have mostly been reported in Section 6. The Ethyl Corporation program uses analytical information provided by the FIA (ASTM D1319) method; at times this was replaced by data from the more detailed analyses. Normal butane was assumed to have a Research Octane Number of 94.0, and a Motor Octane Number of 90.0 [27]. In addition to generating octane number estimates for blends, ESP also calculated distillation quality; this was useful to check whether the formulations were "reasonable" gasolines.

Similar comments apply to the ESP Motor Octane Number predictions. Although here the bias is appreciably larger (+0.67), it disappears in the calculation of MON upon component substitution. The scatter is not significantly greater than for RON. Further details of the statistical evaluations are given in Appendix III.

On the whole, ESP worked very well for the hydrocarbon fuels made up in this project. No attempt was made to develop Octane Number correlations superior to ESP, for purposes of this contract. Hydrocarbon blending values in the LP data base had also been developed with the aid of this technology, and they did not require adjustments. Oxygenate performance is a more controversial matter; this will now be discussed in the sub-section that follows.

8.2 Input Data for Oxygenates and Experimental Study of Alcohol Blending Values

As in the matter of synthetic crude utilization, prices were bound to have a great effect on LP calculations concerning oxygenates. To make oxygenate prices both realistic and compatible with other information in the LP data base, a factor was established between mid-1984 U.S. Gulf Coast prices of propane and n-butane and the prices of these hydrocarbons in the LP. This factor was used to convert estimated mid-1984 U.S. selling prices to Canadian supply costs. As for the U.S. prices, they were developed primarily on the basis of Penny and Andre's economic analysis [15]. The preceding approach implicitly assumed that oxygenates would eventually be manufactured in Canada on a large scale. For purposes of a sensitivity study, higher methanol and gasoline-grade tertiary butyl alcohol (GTBA) prices were also considered, based on a Canadian methanol cost of 18.0 ¢/L and adding transportation costs, duty and exchange to the U.S. price of GTBA [28].

The conclusions of the economic evaluations will not be greatly affected by the sharp fluctuations we experience in crude prices, because - in the first approximation - hydrocarbon and oxygenate prices move up and down proportionately. For example, Reference 15 points out that GTBA production costs are determined primarily by the price of isobutane.

The most relevant unit prices used in the LP evaluations are shown in Table 8.3. No price sensitivity studies were conducted for MTBE, since the economics of the latter product were more thoroughly considered in another contract (see Section 3).

Turning to blending values, it should be noted that, in the words of one reviewer [29], the alcohols "do not mix well" with gasoline hydrocarbons. This gives rise to a very high, non-linear increase in vapour pressure, octane improvement is greatly dependent on base fuel composition - and perhaps on driving conditions -, water tolerance is problematic, etc. MTBE-hydrocarbon blends behave much more ideally (in the physico-chemical sense) but the blending octanes are still variable [28, 30].

As mentioned earlier, in view of the overlap with another contract, the LP evaluation of MTBE was not extensive here. Sensitivity studies were limited to the consideration of three sets of blending octanes*: RON = 129, MON = 98 (a very favourable Road Octane performance [30]); RON = 119, MON = 97 (suggested by Reference 28); and RON = 112, MON = 93, representing moderate response [30].

Because of the considerable uncertainties in alcohol blending values, most of the LP runs dealt with different combinations of Oxinol 50 vapour pressure and anti-knock effects. For the low-price case, all possible combinations of low and high blending vapour pressures with low and high blending octanes were explored. The initial input data are shown in Table 8.4. For both the high and low vapour pressure cases, blending RVP is given as a function of oxygenate concentration; it is seen that small amounts of Oxinol 50 will displace disproportionately large quantitites of butane. This is not the only drawback of low alcohol concentrations; water tolerance greatly improves when increasing amounts of Oxinol 50 are added to the base fuel [31]. Specifications were set up in a manner to ensure that 1000 ppm by weight of water would remain miscible with the oxygenated fuels in any season. After simplification, this suggested minimum Oxinol 50 contents of 5 volume % April through September and 7 volume % during the other six months. For the high-price Oxinol 50 "scenario", only the low octane-low vapour pressure combination was evaluated, with the same minimum concentrations stipulated.

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*at zero manganese additive level.

Finally, it was necessary to estimate the octane improvement that could be achieved by the use of manganese additive (MMT) - allowed in both hydrocarbon and oxygenated fuels. The manganese response was expected to be higher in regular than in premium gasolines; this is reflected in the input data of Table 8.5.

Results of the LP evaluations will be discussed mostly in Section 9; but they have also suggested oxygenated gasoline compositions suitable to determine blending values experimentally. (The experimental studies were limited to Oxinol 50 as the oxygenate; once again, to avoid duplication of effort with another contract.) Appendix IV gives considerable detail on the blend design, and Table 8.6 shows the resulting formulations.

Most of the required fuel components had been used in the previous blending studies (Section 8.1), but it was desirable to confirm that they were still in good condition. Indeed, the wide-range Port Moody cat. cracked gasoline was found to be badly weathered; so, it was replaced by a similar sample from Petro-Canada's Trafalgar Refinery. Recent inspections of the fuel components used to prepare the sub-octane base gasolines are given in Table 8.7. Both the base and oxygenated gasolines were treated with manganese additive, as per the blend design.

Determining the vapour pressure and knock resistance of the sub-octane hydrocarbon fuels and oxygenated gasolines, did furnish significant new information. The octane data are given in Table 8.8 and show that Oxinol 50 blending octanes may be much lower than generally thought - especially for Motor Octane. It is confirmed that octane appreciation is very dependent on base gasoline composition. (There is no evidence, however, that the substitution of Syncrude heavy reformate and Udex raffinate for conventional reformates and light straight run gasoline has significantly affected the Oxinol 50 blending values.) The results suggest a sensitivity study with Oxinol 50 blending values of 113 for RON and 83 for MON at the zero manganese level*. The

*From Table 8.8, RON = 113.8 is the low-level blending octane that can be calculated the most accurately. This result corresponds to Gasoline G5 (Regular Unleaded, 0.03 gram MMT/U.S. gallon). Correcting for manganese response (Table 8.5), we get RON = 112.8. This value was rounded up to 113. The MON response to Oxinol 50 was very small for gasolines G4 and G5, hence the blending sensitivity was taken to be the round number 30, giving a blending MON of 83. This is consistent with the experimental results on Gasolines G4 and G5.

data also confirm the expected dependence of incremental vapour pressure on oxygenate concentration (Table 8.9). Here, the deviations between assumed and observed RVP blending values are not great. One might speculate that the high alkylate content of gasoline G1 has increased the solubility of butane, and that this is responsible for the low blending RVP of Oxinol 50 in the latter formulation. However, further sensitivity analysis is hardly warranted on the basis of Table 8.9.

It now appears that the strengths and weaknesses of various types of input parameters into the LP evaluations have been adequately considered. Bearing in mind the uncertainties, the section that follows will present the main findings of the LP studies.

9. RESULTS OF THE LINEAR PROGRAMMING EVALUATIONS

Overall, the LP studies have indicated that oxygenates will be economically attractive in the no-lead environment of the future. This is in agreement with another recent, Canadian LP analysis [28], albeit the two studies have used different approaches.

MTBE utilization suggested by the LP was always at the maximum allowed level (11 vol.%, see Reference 30) for premium unleaded and at the 3-4 volume % level (annual average) for regular unleaded gasolines - the higher usage corresponding to higher blending octanes assumed. The main driving force that leads to cost savings with MTBE is the reduction of C_5/C_6 naphtha sales by one-third. This, plus the incorporation of MTBE, reduce crude costs by approximately 7%. (Oxygenates allow increased synthetic crude utilization, as well as reducing the total crude volume processed.) The savings are not strongly dependent on MTBE blending octanes - within the range covered by the studies (RON from 112 to 129, MON from 93 to 98). The use of MTBE also leads to lower manganese antiknock and reforming costs; here, the results are more sensitive to MTBE blending octanes, see Table 9.1. (The latter table shows the overall savings with MTBE as a percentage of the total variable costs of the base case - no oxygenates.)

Although MTBE economics appear to be relatively independent of the blending octanes, undoubtedly they would be highly dependent on MTBE production costs. For instance, a recent study under another

contract [33] concluded that MTBE production was less attractive from refinery C_4 olefins than to upgrade the latter by alkylation. Because of the overlap with this other contract, MTBE economics were not pursued any further in the present work.

The main thrust of the linear programming evaluations was to assess the economics of methanol-cosolvent octane appreciators, specifically methanol-tertiary butyl alcohol (Oxinol 50), the system whose technology is the best established [10]. This involved sensitivity studies with respect to Oxinol 50 price, blending octanes and blending Reid vapour pressures. As mentioned in Section 8.2, experimental studies based on the first set of LP calculations suggested the need for a further evaluation: would Oxinol 50 be attractive at lower blending octanes (especially in terms of Motor and Road Octane) than usually assumed? Results of the latter analysis will be included in the discussion that follows.

First, it is significant that even at a rather high alcohol price (32.84¢/L, see Table 8.3) Oxinol 50 offered some economic advantages compared to the base case (no oxygenates). However, the savings were quite small (0.37% of the total variable cost), and so was the amount of Oxinol 50 blended into gasolines. The premium unleaded gasolines were formulated with the maximum concentration of Oxinol 50 allowed (10 volume %), but alcohols were absent from the regular unleaded gasolines. As with MTBE, the driving force was reduced naphtha sales and crude purchases, but at levels 60% lower than for MTBE. There was no reduction in reforming severity or in manganese antiknock purchases compared to the (oxygenate-free) base case (see Table 9.2).

Turning to low-priced Oxinol 50 (24.93¢/L, see Table 8.3), sensitivity studies were carried out with respect to blending octanes and vapour pressures. These were in the nature of a factorial experiment: all possible combinations of "low" and "high" vapour pressures with three octane levels (Table 8.4 plus the RON = 113, MON = 83 cases) were explored. Persisting with statistical terminology, one might say that the vapour pressure and octane main effects were relatively small, and that the RVP-ON interactions were unimportant. Certainly, even a glance at Table 9.2 suggests that quantitative uncertainties in antiknock and volatility performance are not all that critical. The role of oxygenate

price is much more pronounced. As mentioned in Section 1, materials/fuel compatibility and product handling may be the significant potential technical problems [11]. Although the volatility and octane improver performance of oxygenated motor fuel components is not known precisely - there are insufficient data and the relevant theories are not well developed -, these matters do not seem to deserve concentrated attention at the present time. One would be inclined to go even a step further. Prices may not be the most critical factor either (they could be lowered, given sufficient demand), but rather the environmental considerations mentioned in Section 1. However, the latter thoughts are more in the nature of overall conclusions, leading up to Section 10, which follows.

10. CONCLUSIONS

10.1 The Resource Base for Gasoline Production in Canada at the End of the Twentieth Century

A review of recent developments and current trends in the petroleum industry suggests that the utilization of heavy oil and tar sand resources will increase in Canada by the end of this century. Linear programming evaluations conducted under the present project have revealed no serious barriers to 25% synthetic crude in the crude slates of Canadian refineries.

Among other "novel" sources of spark ignition engine fuels, natural gas deserves the most attention. Natural gas is presently the most economical feedstock for methanol production, and the latter chemical has potential as a motor fuel by itself, can be blended into gasoline with cosolvents, reacted with olefins to yield high-octane ethers, or it can be converted to gasoline, e.g. via the Mobil MTG process. The natural gas-acetylene-ethylene-gasoline route may be even more attractive economically. (Natural gas itself can also be used as an automotive fuel, but this opens up a subject for discussion that is outside the scope of the present contract.)

Propane and butane supplies (from both refinery and natural gas sources) are adequate to serve as raw materials for a number of oxygenated gasoline components, in particular methyl tertiary butyl ether (MTBE) and cosolvent alcohols (to be used with methanol). The aromatization of propane and butanes (BP-UOP Cyclar Process) could be equally or yet more promising.

At the other end of the spectrum of potential gasoline precursors are coal and shale oil. Neither of them is likely to be a significant factor in Canadian motor fuel production over the next 15 years. Nor does it seem likely that ethanol, produced from renewable resources, will make major inroads into the Canadian gasoline markets - unless by legislation.

10.2 Gasoline Composition and Properties - Conclusions Drawn from the Experimental Program

Dwindling conventional crude reserves not only favour increased utilization of heavy oil and tar sands, but also suggest "cutting deeper into the barrel" - residuum upgrading. Declining demand for heavy fuel oils is accelerating the latter trend. Gradual elimination of lead antiknock compounds has led to widespread use of high-severity reforming and isomerization of light straight run gasoline. These developments, however, are not causing fundamental changes in the composition of gasolines. In the present project, it was found that current procedures for estimating the octane numbers of hydrocarbon fuels remain valid when "synthetic" streams are substituted for conventional fractions.

The elimination of lead antiknocks is also a powerful driving force for a more revolutionary change in spark ignition fuels: incorporation of up to (approximately) 10 volume % of oxygen containing organic compounds. The properties of the resultant fuel mixtures are dependent on the base gasoline composition and are often not well known. Blending studies with Oxinol 50 (50 volume % methanol-50 volume % tertiary butyl alcohol), conducted under the present project, suggest that the latter octane appreciator may well blend at a Road Octane as low as 98 or as high as 113. Blending vapour pressures are also subject to variations (especially with oxygenate concentration), but they were found to be in acceptable agreement with estimates published in the literature.

Detailed compositional analysis of gasoline streams can reveal correlations between fuel properties and the processing scheme. For instance, the high end points (approximately 260°C) of heavy Syncrude reformates appear to be caused by the presence of multi-substituted benzene derivatives, prevalent in synthetic crudes.

10.3 Linear Programming Results; Conclusions of the Sensitivity Studies

The fundamental conclusion of LP evaluations was that MTBE and Oxinol 50 both were economically attractive in a no-lead environment.

For MTBE, the sensitivity analysis covered a fairly narrow (though realistic) range of blending octanes; within this range the economics were not strongly dependent on the precise octane response. (However, small differences could be crucial in choosing between different approaches, e.g. isomerization versus MTBE purchase.)

Oxinol 50 sensitivity studies explored the roles of additive price, blending octanes and blending vapour pressures. The use of Oxinol 50 was found economical in all cases. Savings as percentages of the total variable cost without oxygenates were relatively independent of the blending values but were strongly depressed when the unit price of Oxinol 50 was raised from 25¢/L to 33¢/L (approximately).

As discussed in Section 8.2, absolute costs will change with movements in crude prices, but relative costs - and hence the preceding conclusions - will not be greatly affected.

10.4 Overall Assessment

Among "novel" sources of spark ignition engine fuels, heavy oil/tar sands and natural gas deserve the most attention in Canada. There is much controversy surrounding the conversion of natural gas to automotive gasolines; it is difficult to predict what form it will take and how much it will cost. Probably environmental concerns will decide the issue eventually, rather than what is currently known about natural gas - gasoline processes and the performance of their products.

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TABLE 4.1

Pilot Plant Reforming of Syncrude Light Naphtha

Run No.	Operating Temperature °C	Product		
		API Gravity	RON Clear	MON Clear
01	474	45.2	96.6	83.8
02	460	48.6	90.4	77.4

TABLE 4.2

Reformer Material Balances, Syncrude Light Naphtha

Run#01 BASIS:1HR

FEEDRATE: 173.68 g/hr HC
13.24 g/hr H2 (4:1 H2/HC)

186.92 g/hr Total Feed

PRODUCT: 43.89 g/hr Reaction gas
12.4 H2
2.04 C1
3.44 C2
7.09 C3
10.49 C4
8.43 C5+
136.76 g/hr Gasoline

180.65 g/hr Total Product

Material Balance= 96.64562 %
Total C5+ Losses= 5.896184 %
Corrected C5+ Yield= 83.59626 % C5+ RON= 96.6

Run#02 BASIS:1HR

FEEDRATE: 177.6 g/hr HC
13.54 g/hr H2 (4:1 H2/HC)

191.14 g/hr Total Feed

PRODUCT: 29.93 g/hr Reaction gas
11.46 H2
0.91 C1
1.58 C2
4.4 C3
6.63 C4
4.95 C5+
155.44 g/hr Gasoline

185.37 g/hr Total Product

Material Balance= 96.98127 %
Total C5+ Losses= 3.086227 %
Corrected C5+ Yield= 90.30968 % C5+ RON= 90.4

TABLE 4.3

Reformer Material Balances, Syncrude Heavy Naphtha

FEED COMPOSITION	vol%		UNIT CONDITIONS	
Paraffins	37.13		LHSV	1.5
iso-		25.58	TEMP.,C	500,483
n-		11.54	PRESS.,psi	340
Naphthenes	47.46		H2/HC	4:1
Aromatics	15.41			
RON:	85			

Run#80 BASIS:1HR

FEEDRATE: 177.85 g/hr HC
10.54 g/hr H2 (4:1 H2/HC)

PRODUCT: 67.22 g/hr Reaction gas
10.02 H2
8.16 C1
12.74 C2
15.47 C3
14.62 C4
6.21 C5+
122.7 g/hr Gasoline

188.39 g/hr Total Feed

189.92 g/hr Total Product

Material Balance= 100.8121 %
Total C5+ Losses= 4.817314 %
Corrected C5+ Yield= 72.48242 % C5+ RON= 102.8

Run#81 BASIS:1HR

FEEDRATE: 176.98 g/hr HC
10.49 g/hr H2 (4:1 H2/HC)

PRODUCT: 56.88 g/hr Reaction gas
11.44 H2
5.94 C1
7.75 C2
10.47 C3
11.77 C4
9.49 C5+
130.72 g/hr Gasoline

187.48 g/hr Total Feed

187.58 g/hr Total Product

Material Balance= 100.0893 %
Total C5+ Losses= 8.768418 %
Corrected C5+ Yield= 79.23259 % C5+ RON= 97

REFORMER YIELD CURVE: SYNCRUDE HVY. NAPHTHA

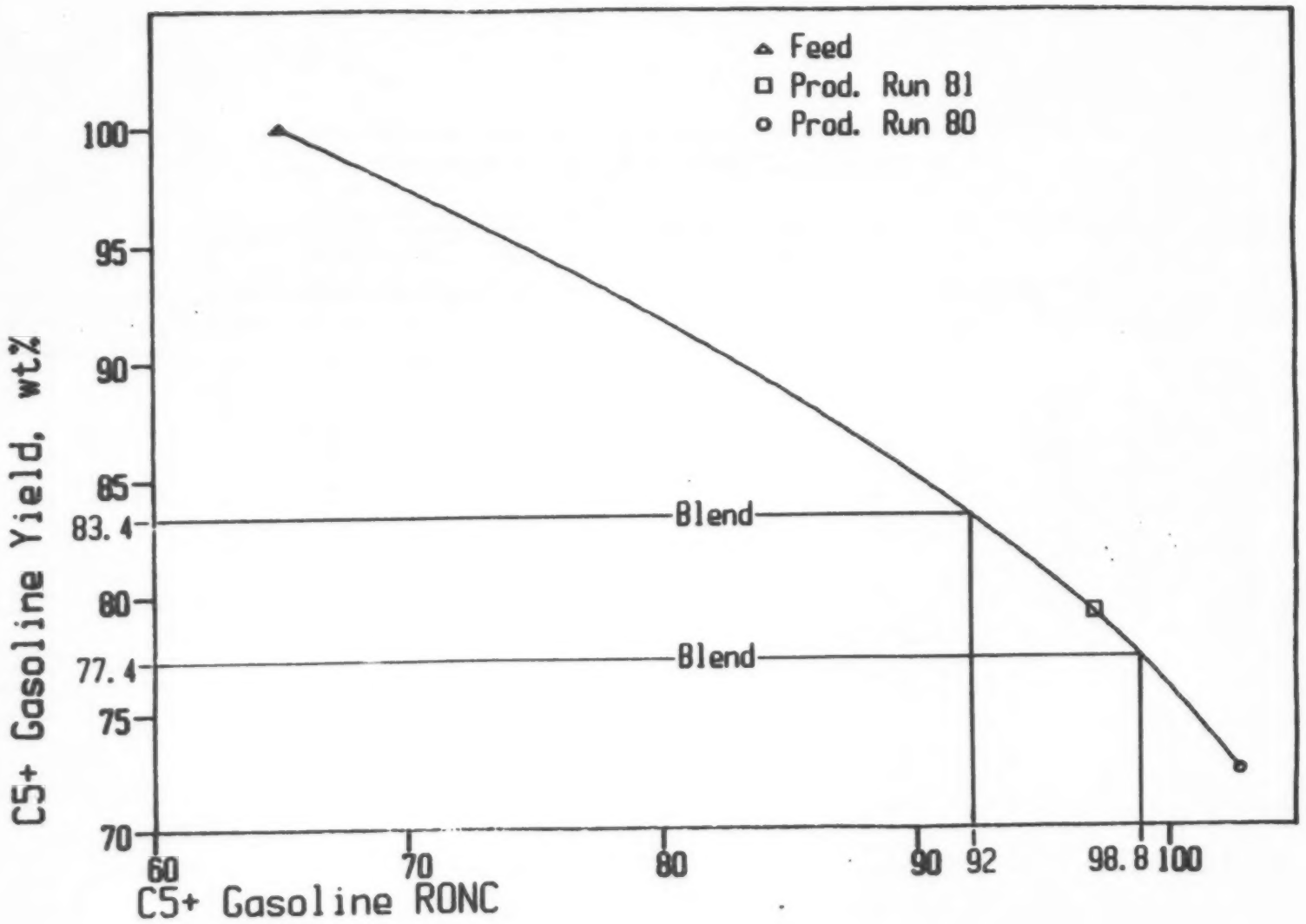

Figure 4.1

TABLE 6.1

Inspections of Conventional Gasoline Component Samples, Acquired (or Prepared) for Blending Studies

Sample:		P.R.* Prefractionator Overhead	P.R. Light Reformate, Nominal 77 RON Clear	P.R. Light Reformate, Nominal 85 RON Clear	P.R. Heavy Reformate, Nominal 90 RON Clear	P.R. Heavy Reformate, Nominal 97 RON Clear	P.R. Wide-Range Cat. Cracked Gasoline	P.R. FCCU IBP-80°C Cut	P.R. FCCU 80-140°C Cut	P.R. FCCU 140°C+ Cut	P.R. C_6 Alkylate	Mtl.* Udex Raffinate	Mtl. Polymerization Gasoline	Trafalgar* Wide-Range Cat. Cracked Gasoline
Sample No.:		P.G.E.	D85-110	D85-116	D85-119	D85-117	D85-120	D85-120-1	D85-120-2	D85-120-3	D85-121	D85-115	MR-54-1	R&D 81252
Reid Vapour pressure, kPa (psi),	ASTM D-323	91.9(13.3)	22.1(3.2)	14.5(2.1)	18.7(2.7)	22.1(3.2)	68.4(9.9)	150.6(21.8)	4.5(0.65)	NIL	54.6(7.9)	27.6(4.0)	69.1(10.0)	36.6(5.3)
Gravity, °API,	ASTM D-287	83.1	54.2	53.6	47.5	44.0	59.6	84.1	53.8	35.7	71.7	69.2	64.3	55.7
Distillation, °C at volt evaporated,	ASTM D-86													
IBP		30	55	60	61	64	38	22	93	154	32	56	31	41
10%		38	79	73	97	88	66	37	102	162	55	70	90	58
20%		41	85	88	111	104	55	32	104	166	72	74	100	67
30%		44	89	87	120	115	49	36	106	169	90	78	112	78
40%		47	94	98	127	125	86	41	108	173	101	82	113	92
50%		50	100	98	133	132	101	46	111	177	106	86	114	109
60%		55	105	104	139	139	118	50	114	183	110	91	116	127
70%		60	112	111	145	146	130	55	118	187	114	98	120	147
80%		67	118	119	151	152	159	60	122	194	120	106	131	166
90%		76	129	130	159	162	182	67	125	204	150	120	160	186
FBP		94	150	156	188	190	212	86	141	225	215	167	201	213
Recovery		96.5	99.0	99.0	98.7	99.5	97.0	98.0	98.8	98.4	98.6	99.3	97.0	97.8
Residue		0.6	0.3	0.4	0.2	0.2	0.3	0.5	0.1	0.4	0.5	0.7	0.4	0.4
Loss		0.9	0.6	0.6	0.1	0.2	2.6	1.5	0.1	0.2	0.9	0.4	2.6	1.8
Sulfur, wt.%,	ASTM D3622	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	0.01	0.06	0.01	<0.01	<0.01	0.07
Research Octane Number (Clear)	ASTM D2699	74.8	83.0	87.8	97.3	97.1	Not determined	94.9**	87.4	98.1	93.5	84.2	98.5	90.4
Motor Octane Number (Clear)	ASTM D2700	72.7	77.2	79.6	78.9	86.4	Not determined	82.6	78.8	88.7	91.2	82.8	83.5	80.1

*P.R. = Petro-Canada's Port Moody Refinery
Mtl. = Gulf Canada's Montreal East Refinery
Trafalgar = Petro-Canada's Oakville Refinery

** Vapour locking encountered

TABLE 6.2

Inspections of Light and Heavy Syncrude Reformates Produced in the Pilot Plant

		Syncrude Light Reformate		Syncrude Heavy Reformate	
		96.6 RON(clear)	90.4 RON(clear)	92.0 RON(clear)	98.8 RON(clear)
Sample No.:		86-P12-003	86-P12-002	85-P12-074	85-P12-075
Reid Vapour pressure, kPa (psi),	ASTM D-323	19.3 (2.8)	18.0 (2.6)	9.7 (1.4)	11.1 (1.6)
Gravity, °API,	ASTM D-287	45.2	48.6	39.3	35.6
Distillation, °C	ASTM D-86				
at vol% evaporated					
IPB		54	60	49	50
10%		85	88	110	110
20%		90	92	132	133
30%		97	97	144	144
40%		102	101	153	152
50%		107	105	159	158
60%		113	110	165	165
70%		119	116	173	173
80%		125	122	182	182
90%		134	132	197	200
FBP		168	163	253	265
Recovery		99.2	99.2	99.0	99.3
Residue		0.6	0.7	0.5	0.6
Loss		0.2	0.1	0.5	0.1
Motor Octane Number (Clear)	ASTM D2700	83.8	77.4	82.1	87.4

TABLE 6.3

Inspections of Light, Intermediate and Heavy Cat. Cracked Gasoline* Fractions ex Murphy Oil's Meraux, Louisiana Refinery

Sample:		IBP-80°C	80-140°C	140°C+
Reid vapour pressure, kPa (psi),	ASTM D-323	116.1 (16.8)	7.6 (1.1)	0
Gravity, °API,	ASTM D-287	80.1	51.5	36.8
Distillation, °C at vol% evaporated,	ASTM D86			
IBP		24	94	155
10		29	102	165
20		33	104	168
30		37	105	172
40		41	108	175
50		46	111	179
60		51	114	183
70		56	118	188
80		62	124	195
90		69	131	204
FBP		87	158	219
Recovery		95.7	99.5	99.2
Residue		0.5	0.4	0.7
Loss		3.8	0.1	0.1
Sulfur, wt.%,	ASTM D-2622	0.00	0.04	0.08
Research Octane Number (clear)	ASTM D-2699	95.2	90.4	88.4
Motor Octane Number (clear)	ASTM D-2700	81.0	78.3	79.3

* Crude: 40-50% North Sea (Forties), 50-60% Louisiana Sweet. The feed charged to the FCCU contained 60-70% residuum. An implementation of UOP's RCC (Residual Catalytic Cracking, see Reference 22) process.

TABLE 6.4

COMPOSITIONAL ANALYSIS OF GASOLINE BLENDING COMPONENTS

Conventional & Synthetic Reformates

COMPONENT	Light Reformates				Heavy Reformates			
	P.M. 118	P.M. 116	Syncr 002	Syncr 003	P.M. 119	P.M. 117	Syncr 074	Syncr 075
	Summary of GC & MS Analytical Data (Liquid Volume %)							
P (C4-C12 n/isoP)	57.5	55.1	45.4	37.6	51.3	41.3	40.8	28.6
I (C4-C12 isoPar)	39.2	37.3	32.2	26.6	31.6	27.6	24.0	17.0
N (C4-C12 n-Par)	18.3	17.8	13.2	11.0	19.7	13.7	16.7	11.7
C (C5-C12 Cy-Par)	4.0	2.7	6.4	2.9	4.1	2.4	12.9	8.7
A (C6-C12 Aromatics)	38.5	42.3	48.2	59.6	44.6	56.3	46.4	62.7
TOTAL	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
Calc. Average M.W.	95.9	93.8	96.6	95.3	106.7	103.6	111.7	109.8
MON	77.2	79.6	77.4	83.8	78.9	86.4	82.1	87.4
RON	83.0	87.8	90.4	96.6	87.3	97.1	92.0	98.8
% OFF	DISTILLATION DATA (ASTM D86) Deg C							
IBP	55	49	54	60	61	64	49	50
10	79	73	85	88	97	88	110	110
20	85	81	90	92	111	104	132	133
30	89	87	97	97	120	115	144	144
40	94	92	102	101	127	125	153	152
50	100	98	107	105	133	132	159	158
60	105	104	113	110	139	139	165	165
70	112	111	119	116	145	146	173	173
80	118	119	125	122	151	153	182	182
90	129	130	134	132	159	162	197	200
FBP	150	156	168	163	180	190	253	265
Reid Vapour Pressure, kPa	22.1	14.5	18.0	19.3	18.7	22.1	9.7	11.1
API Gravity	54.2	53.6	48.6	45.2	47.5	44.0	39.3	35.6

TABLE 6.4 (continued)

COMPOSITIONAL ANALYSIS OF GASOLINE BLENDING COMPONENTS

Conventional & Synthetic Reformates

COMPONENT	Light Reformates				Heavy Reformates			
	P.M. 118	P.M. 116	Syncr 002	Syncr 003	P.M. 119	P.M. 117	Syncr 074	Syncr 075
	MASS SPECTROMETRIC COMPOSITIONAL ANALYSIS (LV%)							
Benzene	5.5	6.5	5.7	7.7	2.0	2.9	1.0	1.5
Toluene	17.8	19.4	23.5	27.7	9.6	12.1	5.3	7.8
C8 Aromatics	13.1	14.2	17.4	20.6	16.4	20.5	14.5	19.3
C9 Aromatics	2.1	2.3	1.7	2.9	14.0	17.8	15.7	20.7
C10 Aromatics				0.6	2.3	2.9	7.7	9.8
C11 Aromatics							0.7	1.3
C12 Aromatics								
Indans + Tetralins					0.2	0.2	1.5	2.4
Naphthalenes								
C6-C12 Aromatics	38.5	42.3	48.2	59.6	44.6	56.3	46.4	62.7
C6 Paraffins	19.2	20.1	9.9	13.1	4.4	7.0	5.9	3.4
C7 Paraffins	21.9	19.0	22.4	17.7	10.6	10.6	5.8	2.7
C8 Paraffins	12.3	8.8	10.8	3.5	15.3	10.9	8.0	3.0
C9 Paraffins					13.2	6.2	10.8	10.1
C10 Paraffins					3.2		4.6	3.7
C11 Paraffins								
C12 Paraffins								
Total C6-C12 Par	53.4	47.9	43.2	34.4	46.6	34.8	35.1	22.9
C6C12 Isoparaffins	41.0	38.2	38.2	31.8	40.1	33.3	35.1	18.3
C6-C12 n-Paraffins	12.4	9.7	5.1	2.6	6.5	1.5		4.6
Total n- + iso-Par	53.4	47.9	43.2	34.4	46.5	34.8	35.1	22.9
C5 Cycloparaffin	0.3	0.4	0.1	0.1	0.1	0.1	0.2	0.2
C6 Cycloparaffins	1.9	1.2	3.7	1.1	1.7	0.9	2.3	1.1
C7 Cycloparaffins	1.2	0.6	2.0	1.4	1.2	0.6	2.1	0.9
C8 Cycloparaffins	0.6	0.4	0.5	0.3	0.7	0.5	3.1	1.0
C9 Cycloparaffins					0.3	0.2	1.8	3.3
C10 Cycloparaffins							1.5	1.2
C11 Cycloparaffins								
C12 Cycloparaffins								
Total C5-C12 CyPar	3.9	2.5	6.3	2.8	3.9	2.3	11.0	7.6
C5+ Cyclopentanes	2.9	1.8	4.9	2.0	2.2	1.4	5.1	5.9
C5+ Cyclohexanes	1.0	0.7	1.4	0.8	1.7	0.9	5.9	1.7
C5+ Cycloparaffins	3.9	2.5	6.3	2.8	3.9	2.3	11.0	7.6
C8+ Dicycloparaffins	0.2	0.1	0.1	0.1	0.2	0.1	1.8	1.0
Total	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0

COMPOSITIONAL ANALYSIS OF GASOLINE BLENDING COMPONENTS

TABLE 6.4 (continued)
Conventional & Synthetic Reformates

COMPONENT	Light Reformates				Heavy Reformates			
	P.M. 118	P.M. 116	Syncr 002	Syncr 003	P.M. 119	P.M. 117	Syncr 074	Syncr 075
SUMMARY of GC CAPILLARY ANALYSES (LV%)								
C4 n-Paraffin	0.5	2.0	0.3	0.3	1.1	0.5	0.7	0.5
C5 n-Paraffin	1.4	2.1	0.7	1.3	1.3	2.5	1.7	1.8
C6 n-Paraffin	6.6	6.3	4.2	4.2	2.1	2.5	1.7	1.8
C7 n-Paraffin	5.3	4.1	4.4	3.1	2.6	1.8	0.9	0.6
C8 n-Paraffin	1.9	1.2	1.6	0.6	2.7	1.2	1.1	0.6
Total C4-C8 n-Par	15.7	15.7	11.1	9.5	9.8	8.6	6.0	5.3
C4 iso-Paraffins	0.0	.0	0.1	0.1	0.3	.0	0.1	0.1
C5 iso-Paraffins	2.3	3.3	1.3	1.9	1.8	3.6	1.7	1.8
C6 iso-Parafins	11.4	12.7	6.6	9.3	3.5	5.7	3.2	3.6
C7 iso-Paraffins	14.7	13.3	14.6	10.7	5.8	6.3	2.8	2.2
C8 iso-Paraffins	7.2	5.0	6.6	2.5	7.5	5.3	2.8	1.5
Total C4-C8 isoPar	35.6	34.4	29.2	24.5	18.8	20.9	10.7	9.2
C4 n-Par + iso-Par	0.5	2.1	0.4	0.4	1.4	0.6	0.8	0.7
C5 n-Par + iso-Par	3.6	5.3	2.0	3.3	3.1	6.2	3.4	3.6
C6 n-par + iso-Par	18.0	19.0	10.7	13.6	5.6	8.2	4.9	5.3
C7 n-Par + iso-Par	20.0	17.5	19.0	13.7	8.4	8.2	3.7	2.8
C8 n-Par + iso-Par	9.1	6.3	8.2	3.1	10.2	6.5	3.9	2.0
Total C4-C8 n/isoP	51.3	50.1	40.4	34.0	28.6	29.6	16.7	14.5
C5 Cyclopentane	0.3	0.4	0.0	0.0	0.2	0.2	0.2	0.2
C6 Cyclopentane	1.9	1.1	3.2	1.2	1.0	0.4	0.6	0.3
C7 Cyclopentanes	0.9	0.5	1.5	0.7	1.4	0.3	0.3	0.2
C8 Cyclopentanes	0.3	0.3	0.5	0.1	0.7	0.2	0.5	0.3
Total C5-C8 CyC5's	3.5	2.2	5.2	2.1	3.3	1.1	1.6	1.0
C6 Cyclohexane	0.2	0.1	0.3	0.1	0.1	.0	0.1	.0
C7 Cyclohexane	0.3	0.2	0.5	0.3	0.2	0.1	0.2	0.1
C8 Cyclohexane	0.5	0.3	0.5	0.2	0.6	0.3	0.5	0.3
Total C6-C8 CyC6's	1.0	0.6	1.3	0.6	0.9	0.5	0.7	0.4
C6 Cycloparaffins	2.1	1.2	3.5	1.3	1.0	0.5	0.6	0.4
C7 Cycloparaffins	1.2	0.6	2.0	1.0	1.6	0.4	0.5	0.3
C8 Cycloparaffins	0.9	0.6	1.0	0.3	1.3	0.6	0.9	0.5
C6 Aromatic	6.0	7.1	6.3	8.5	2.1	3.2	0.8	1.5
C7 Aromatic	19.3	21.1	25.7	30.4	10.1	12.2	4.7	7.2
C8 Aromatics	14.1	12.2	20.0	21.8	15.7	16.0	13.6	17.8
Total C6-C8 Aromatics	39.4	40.4	52.1	60.7	27.9	31.5	19.1	26.5
C4 Olefins	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5 Olefins	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C6 Olefins	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total C4 Olefins	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5 Cyclo-olefins	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
P (C4-C8 n/iso-P)	51.3	50.1	40.4	34.0	28.6	29.6	16.7	14.5
I (C4-C8 iso-Par)	35.6	34.4	29.2	24.5	18.8	20.9	10.7	9.2
N (C4-C8 n-Par)	15.7	15.7	11.1	9.5	9.8	8.6	6.0	5.3
O (C4-C6 Olefins)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C (C5-C8 Cy-Par)	4.5	2.8	6.5	2.6	4.2	1.6	2.3	1.4
A (C6-C8 Aromatics)	39.4	40.4	52.1	60.7	27.9	31.5	19.1	26.5
TOTAL	95.1	93.3	99.0	97.4	60.6	62.7	38.1	42.3
GC LIGHT ENDS ANALYSIS (Liqud Volume %)								
Isobutane	0.0	0.1	0.1	0.1	0.4	.0	0.2	0.2
n-Butane	0.5	2.0	0.3	0.3	1.2	0.6	0.9	0.8
Isopentane	2.2	3.1	1.2	1.7	1.8	3.5	2.4	2.5
n-Pentane	1.4	1.9	0.6	1.1	1.3	2.4	2.2	2.4
Total C4-C5 n/isoP	4.1	7.1	2.2	3.2	4.8	6.6	5.6	5.7
Cyclopentane	0.3	0.4	0.1	0.1	0.1	0.1	0.2	0.2
Total Lt. Ends	4.3	7.5	2.2	3.2	4.9	6.6	5.9	5.9

COMPOSITIONAL ANALYSIS OF GASOLINE BLENDING COMPONENTS

TABLE 6.4 (continued)
Conventional & Synthetic Reformates

COMPONENT			Light Reformates				Heavy Reformates			
			P.M. 118	P.M. 116	Synor 002	Synor 003	P.M. 119	P.M. 117	Synor 074	Synor 075
DETAILED GC CAPILLARY ANALYSIS (Liquid Vol %)										
Isobutane	C4	i-P		.0	0.1	0.1	0.3	.0	0.1	0.1
n-Butane	C4	n-P	0.5	2.0	0.3	0.3	1.1	0.5	0.7	0.5
2,2-Dimethyl-C3	C5	i-P								
Isopentane	C5	i-P	2.3	3.3	1.3	1.9	1.8	3.6	1.7	1.8
N-Pentane	C5	n-P	1.4	2.1	0.7	1.3	1.3	2.5	1.7	1.8
2,2-Dimethylbutane	C6	i-P	0.9	1.0	0.5	0.8	0.2	0.5	0.1	0.2
Cyclopentane	C5	CyP	0.3	0.4			0.2	0.2	0.2	0.2
2,3-Dimethylbutane	C6	i-P	1.0	1.2	0.6	1.0	0.3	0.5	0.3	0.3
2-Methylpentane	C6	i-P	5.4	6.0	3.0	4.3	1.7	2.6	1.6	1.7
3-Methylpentane	C6	i-P	4.1	4.5	2.4	3.3	1.3	2.0	1.2	1.3
N-Hexane	C6	n-P	6.6	6.3	4.2	4.2	2.1	2.5	1.7	1.8
22-Dimethylpentane	C7	i-P	0.6	0.5	0.7	0.5	0.2	0.3	0.1	0.1
Methylcyclopentane	C6	CyP	1.9	1.1	3.2	1.2	1.0	0.4	0.6	0.3
2-4Dimethylpentane	C7	i-P	0.8	0.8	0.7	0.5	0.3	0.4	0.2	0.1
223-Tri-Me-butane	C7	i-P	0.1	0.1	0.1	0.1		.0		
Benzene	C6	A	6.0	7.1	6.3	8.5	2.1	3.2	0.8	1.5
3,3-Di-Me-pentane	C7	i-P	0.6	0.5	0.6	0.5	0.2	0.3	0.1	0.1
Cyclohexane	C6	CyH	0.2	0.1	0.3	0.1	0.1	.0	0.1	.0
2-Methylhexane	C7	i-P	4.8	4.3	4.7	3.4	1.9	2.0	1.0	0.7
2,3Dimethylpentane	C7	i-P	1.6	1.5	1.6	1.2	0.6	0.7	0.3	0.2
11DiMeCyclopentane	C7	CyP	0.1	0.1	0.2	0.1	0.9	.0	0.1	.0
3-Methylhexane	C7	i-P	5.8	5.2	5.6	4.1	2.4	2.4	1.1	0.9
t1,3-Di-Me-CyC5ane	C7	CyP	0.2	0.1	0.3	0.2	0.1	.0	0.1	.0
c1,3-Di-Me-CyC5ane	C7	CyP	0.2	0.1	0.3	0.2	0.1	0.1	0.1	.0
3-Ethylpentane	C7	i-P	0.6	0.5	0.5	0.4	0.2	0.2	0.1	0.1
t1,2-Di-Me-CyC5ane	C7	CyP	0.2	0.1	0.4	0.2	0.2	0.1	0.1	0.1
n-Heptane	C7	n-P	5.3	4.1	4.4	3.1	2.6	1.8	0.9	0.6
Methylcyclohexane	C7	CyH	0.3	0.2	0.5	0.3	0.2	0.1	0.2	0.1
2,2-Dimethylhexane	C8	i-P	0.3	0.2	0.4	0.1	0.3	0.2	0.1	0.1
Ethylcyclopentane	C7	CyP	0.1	0.1	0.3	0.1	0.1	.0	0.1	.0
2,5-Dimethylhexane	C8	i-P	0.5	0.3	0.4	0.2	0.4	0.3	0.2	0.1
2,4-Dimethylhexane	C8	i-P	0.8	0.5	0.6	0.3	0.7	0.5	0.2	0.1
ctc124TriMeCyC5ane	C8	CyP	.0	.0	.0	.0	.0	.0	0.1	.0
2,3,4-Tri-Me-C5ane	C8	CyP	0.3	0.2	0.3	0.1	0.3	0.2	0.1	.0
ctc123TriMeCyC5ane	C8	CyP	.0	.0			.0			
2,3,3-TriMePentane	C8	i-P	.0		.0	.0	.0			
Toluene	C7	A	19.3	21.1	25.7	30.4	10.1	12.2	4.7	7.2
2,3-Dimethylhexane	C8	i-P	0.5	0.4	0.5		0.5	0.6		0.1
2-Me-3-Et-pentane	C8	i-P	0.1		0.1	0.2	0.1		0.2	
2-Methylheptane	C8	i-P	1.8	1.3	1.6	0.6	2.0	1.4	0.7	0.3
4-Methylheptane	C8	i-P	1.2	0.8	1.1	0.4	1.3	0.8	0.4	0.2
3,4-Dimethylhexane	C8	i-P								
cct124TriMeCyC5ane	C8	CyP								
3-Methylheptane	C8	i-P	2.1	1.4	1.9	0.7	2.2	1.4	1.0	0.5
1-Me-2-Et-CyC5ane	C8	CyP								
t-1,4Di-Me-CyC6ane	C8	CyH	0.5	0.3	0.4	0.2	0.5		.0	
1,1DiMeCyclohexane	C8	CyH					0.1	0.3	.0	
c13DiMeCyclohexane	C8	CyH	.0				.0		0.1	0.1
c1-Et-2-Me-CyC5ane	C8	CyP			.0					
c1-Et-3-Me-CyC5ane	C8	CyP			.0				0.1	.0
1Me-t-3-Et-CyC5ane	C8	CyP								
1-Et-1-Me-CyC5ane	C8	CyP	.0	.0	.0		.0		0.1	0.1
t12DiMeCyclohexane	C8	CyH			.0			.0	0.1	.0
ccc123TriMeCyC5ane	C8	CyP								
n-Octane	C8	n-P	1.9	1.2	1.6	0.6	2.7	1.2	1.1	0.6
Isopr-Cyclopentane	C8	CyP								
c12DiMeCyclohexane	C8	CyH								
Ethylcyclohexane	C8	CyH			0.1				0.3	0.2
n-Pr-Cyclopentane	C8	CyP			.0		0.3		0.2	0.1
Ethylbenzene	C8	A	1.9	2.1	2.8	3.3	3.0	3.3	2.2	2.9
m-Xylene	C8	A	6.7	7.2	9.6	11.1	7.9	9.1	5.9	7.9
p-Xylene	C8	A	2.6	2.8	3.4	4.0	3.2	3.3	2.3	2.9
o-Xylene	C8	A	2.8	.0	4.2	3.4	1.6	0.3	3.2	4.1
Total			95.1	93.3	99.0	97.4	60.6	62.7	38.2	42.3

TABLE 6.5

COMPOSITIONAL ANALYSIS OF GASOLINE BLENDING COMPONENTS

Cat. Cracked Gasolines

Summary of Analytical Data (Liquid Volume %)

PM = Port Moody; RCMO = (Resid. Cracked) Murphy Oil

	Full Range		IBP to 80 C		80 C to 140 C		140 C +	
COMPONENT	PM-120	RCMO-915	PM-1201	RCMO-924	PM-1202	RCMO-925	PM-1203	RCMO-926
P (C4-C12 n/isoP)	34.6	20.9	42.7	23.8	29.7	20.7	32.1	24.4
O (C4-C12 Olefins)	25.8	33.5	41.7	58.6	28.2	42.7	7.9	14.0
C (C5-C12 Cy-Par)	22.7	28.7	13.2	13.7	21.5	19.2	25.0	29.9
A (C6-C12 Aromatics)	16.9	16.8	2.3	3.8	20.5	17.1	34.9	32.0
TOTAL	100.0	99.9	99.9	99.9	99.9	99.7	99.9	100.3
Motor Octane Number	80.2	N.D.	82.6	81.0	78.0	78.3	80.7	79.3
Research Octane Number	92.0	N.D.	94.9	95.2	87.4	90.4	90.1	88.4
% OFF	DISTILLATION DATA (ASTM D86) Deg C							
IBP	28		22	24	93	94	154	155
10	44		27	29	102	102	162	165
20	55		32	33	104	104	166	168
30	69		36	37	106	105	169	172
40	84		41	41	108	108	173	175
50	101		45	46	111	111	177	179
60	118		50	51	114	114	182	183
70	138		55	56	118	118	187	188
80	159		60	62	122	124	194	195
90	182		67	69	125	131	204	204
FBP	212		86	87	141	158	225	219
Reid Vapour Pressure, kPa	68	N.D.	151	116	5	8	nil	nil
API Gravity	60	N.D.	84	80	54	52	36	37

N.D. = not determined

COMPOSITIONAL ANALYSIS OF GASOLINE BLENDING COMPONENTS

TABLE 6.5 (continued)

Cat. Cracked Gasolines

Mass Spectrometric Compositional Analyses (Liquid Volume %)

PM = Port Moody; RCMO = (Resid. Cracked) Murphy Oil

	Full Range		IBP to 80 C		80 C to 140 C		140 C +	
COMPONENT	PM-120	RCMO-915	PM-1201	RCMO-924	PM-1202	RCMO-925	PM-1203	RCMO-926
C5 Mono-Olefins	1.7	1.9	4.9	6.4	0.5	0.5	0.2	0.2
C6 Mono-Olefins	8.8	6.6	26.6	34.0	2.0	1.5	0.1	0.3
C7 Mono-Olefins	3.6	5.2	3.1	4.4	7.6	10.1	0.2	0.1
C8 Mono-Olefins	2.6	3.7	0.1	0.2	5.9	8.8	0.2	0.3
C9 Mono-Olefins	1.3	2.3			1.8	3.3	1.5	2.5
C10 Mono-Olefins	0.7	1.2			0.1	0.4	1.4	3.5
C11 Mono-Olefins	0.3	0.4					0.6	1.8
C12 Mono-Olefins	0.3	0.1					0.2	0.5
C13 Mono-Olefins							0.1	
Total	19.3	21.4	34.7	45.0	17.9	24.6	4.5	9.2
C5 Cyclo-Olefins		0.1	0.4	0.3	0.1		0.1	0.1
C6 Cyclo-Olefins	2.0	3.4	5.6	10.5	1.3	2.3	1.5	0.1
C7 Cyclo-Olefins	1.9	3.9	1.0	2.0	4.8	8.3	0.1	0.2
C8 Cyclo-Olefins	1.2	2.2		0.1	2.8	5.0	0.1	0.4
C9 Cyclo-Olefins	0.6	1.2			0.8	1.5	0.7	1.5
C10 Cyclo-Olefins	0.2	0.5			0.1	0.2	0.5	1.5
C11 Cyclo-Olefins	0.1	0.2					0.2	0.7
C12 Cyclo-Olefins	0.1						0.1	0.2
C13 Cyclo-Olefins	0.1						0.1	
Total	6.2	11.5	7.0	12.9	9.9	17.3	3.4	4.7
C5 Dicyclo-Olefins								
C6 Dicyclo-Olefins	0.1	0.2		0.6	0.1	0.1		
C7 Dicyclo-Olefins	0.2	0.4		0.1	0.3	0.7		0.1
C8 Dicyclo-Olefins	0.0							
C9 Dicyclo-Olefins								
C10 Dicyclo-Olefins								
C11 Dicyclo-Olefins								
C12 Dicyclo-Olefins								
C13 Dicyclo-Olefins								
Total	0.3	0.6	0.0	0.7	0.4	0.8	0.0	0.1
C6 Alkyl-benzenes	0.8	0.9	1.5	2.4	0.5	0.5	0.0	0.0
C7 Alkyl-benzenes	2.9	3.3	0.7	0.7	8.5	6.8	0.1	0.0
C8 Alkyl-benzenes	5.6	5.4	0.0	0.2	10.7	8.7	7.1	4.3
C9 Alkyl-benzenes	4.8	4.4	0.0	0.3	0.8	1.0	16.6	14.0
C10 Alkyl-benzenes	1.6	1.6	0.0	0.2	0.0	0.0	7.6	9.1
C11 Alkyl-benzenes	0.2	0.2	0.0	0.0	0.0	0.0	1.2	1.5
C12 Alkyl-benzenes	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1
C13 Alkyl-benzenes								
Total	15.9	15.8	2.2	3.8	20.5	17.0	32.7	29.0
C8 Indans								
C9 Indans	0.2	0.3					0.6	1.0
C10 Indans	0.3	0.3	0.1				1.0	1.9
C11 Indans	0.1	0.1					0.3	0.6
C12 Indans	0.1							0.1
C13 Indans	0.1							
Total	0.8	0.7	0.1	0.0	0.0	0.1	1.9	3.6
C9 Indenes								0.1
C10 Indenes								0.1
C11 Indenes								
C12 Indenes								
C13 Indenes								
Total	0.0	0.1					0.1	
C10 Naphthalenes								0.1
C11 Naphthalenes								
C12 Naphthalenes								
C13 Naphthalenes								
Total	0.0	0.1					0.1	
C12 Biphenyls	0.1	0.1					0.1	0.3
C13 Biphenyls	0.1							0.1
Total	0.2	0.1	0.0	0.0	0.0	0.0	0.1	0.4
Paraffins	34.6	20.9	42.7	23.8	29.7	20.7	32.1	24.4
Mono-cycloparaffins	19.3	21.9	9.8	9.3	19.3	15.9	22.7	22.3
Dicycloparaffins	2.7	5.1	3.1	3.9	1.6	1.9	0.4	4.2
Tricycloparaffins	0.7	1.7	0.3	0.3	0.6	1.4	1.9	3.4
Mono-Olefins	19.3	21.4	34.7	45.0	17.9	24.6	4.5	9.2
Cyclo-Olefins	6.2	11.5	7.0	12.9	9.9	17.3	3.4	4.7
Dicyclo-Olefins	0.3	0.6	0.0	0.7	0.4	0.8	0.0	0.1
Alkylbenzenes	15.9	15.8	2.2	3.8	20.5	17.0	32.7	29.0
Indans	0.8	0.7	0.1	0.0	0.0	0.1	1.9	3.6
Indenes	0.0	0.1	0.0	0.0	0.0	0.0	0.1	0.2
Naphthalenes	0.0	0.1	0.0	0.0	0.0	0.0	0.1	0.2
Biphenyls	0.2	0.1	0.0	0.0	0.0	0.0	0.1	0.4
TOTAL	100.0	99.9	99.9	99.9	99.9	99.7	99.9	100.3

TABLE 6.5 (continued)

COMPOSITIONAL ANALYSIS OF GASOLINE BLENDING COMPONENTS

Cat. Cracked Gasolines

Summary of GC Capillary Analyses (Liquid Volume %)

PM = Port Moody; RCMO = (Resid. Cracked) Murphy Oil

	Full Range		IBP to 80 C		80 C to 140 C		140 C +	
COMPONENT	PM-120	RCMO-915	PM-1201	RCMO-924	PM-1202	RCMO-925	PM-1203	RCMO-926
C4 n-Paraffin	1.3	1.0	2.9	2.2	0.0	0.0	0.0	0.0
C5 n-Paraffin	1.1	0.8	2.6	1.9	0.0	0.0	0.0	0.0
C6 n-Paraffin	0.9	0.6	1.6	1.4	0.3	0.1	0.0	0.0
Total C4-C6 n-Par	3.3	2.4	7.2	5.5	0.3	0.1	0.0	0.0
C4 iso-Paraffins	2.2	0.1	4.9	0.3	0.0	0.0	0.0	0.0
C5 iso-Paraffins	7.1	3.9	16.3	8.8	.0	0.0	0.0	0.0
C6 iso-Parafins	6.7	3.6	14.7	8.4	0.5	0.1	0.0	0.0
Total C4-C6 isoPar	15.9	7.6	35.9	17.4	0.5	0.1	0.0	0.0
C4 n-Par + iso-Par	3.4	1.1	7.8	2.4	0.0	0.0	0.0	0.0
C5 n-Par + iso-Par	8.3	4.7	18.9	10.6	.0	0.0	0.0	0.0
C6 n-par + iso-Par	7.6	4.3	16.3	9.8	0.8	0.2	0.0	0.0
Total C4-C6 n/isoP	19.3	10.1	43.1	22.9	0.8	0.2	0.0	0.0
C5 Cyclopentane	0.1	0.1	0.3	0.3	0.0	0.0	0.0	0.0
C6 Cyclopentane	1.8	1.4	3.4	3.1	1.0	0.6	0.0	0.0
Total C5-C6 CyC5's	1.9	1.5	3.7	3.4	1.0	0.6	0.0	0.0
C6 Cyclohexane	0.1	0.1	0.1	0.1	0.2	0.1	0.0	0.0
C6 Cycloparaffins	1.9	1.5	3.4	3.2	1.2	0.8	0.0	0.0
C6 Aromatic	0.6	0.5	1.0	1.2	0.5	0.4	0.0	0.0
C7 Aromatic	3.1	2.7	0.3	0.3	9.8	8.1	0.0	0.0
C8 Aromatics	4.8	5.4	0.0	0.0	13.4	11.0	7.8	4.5
Total C6-C8 Aromatics	8.5	8.7	1.3	1.5	23.7	19.5	7.8	4.5
C4 Olefins	5.1	6.0	11.6	13.7	0.0	0.0	0.0	0.0
C5 Olefins	8.2	10.9	18.6	24.4	.0	0.0	0.0	0.0
C6 Olefins	5.9	8.2	12.6	18.0	1.5	1.1	0.0	0.0
Total C4-C6 Olefins	19.2	25.1	42.9	56.1	1.5	1.1	0.0	0.0
C5 Cyclo-olefins	0.3	0.6	0.8	1.3	0.0	0.0	0.0	0.0
P (C4-C6 n/iso-P)	19.3	10.1	43.1	22.9	0.8	0.2	0.0	0.0
I (C4-C6 iso-Par)	15.9	7.6	35.9	17.4	0.5	0.1	0.0	0.0
N (C4-C6 n-Par)	3.3	2.4	7.2	5.5	0.3	0.1	0.0	0.0
O (C4-C6 Olefins)	19.2	25.1	42.9	56.1	1.5	1.1	0.0	0.0
C (C5-C6 Cy-Par)	2.0	1.6	3.8	3.5	1.2	0.8	0.0	0.0
A (C6-C8 Aromatics)	8.5	8.7	1.3	1.5	23.7	19.5	7.8	4.6
TOTAL	49.0	45.4	91.0	84.1	27.2	21.6	7.8	4.5

TABLE 6.5 (continued)

COMPOSITIONAL ANALYSIS OF GASOLINE BLENDING COMPONENTS

Cat. Cracked Gasolines

Detailed GC Capillary Analyses (Liquid Volume %)

PM = Port Moody; RCMO = (Resid. Cracked) Murphy Oil

			Full Range		IBP to 80 C		80 C to 140 C		140 C +	
COMPONENT	TYPE		PM-120	RCMO-915	PM-1201	RCMO-924	PM-1202	RCMO-925	PM-1203	RCMO-926
Isobutane	C4	i-P	2.2	0.1	4.9	0.3				
Butene-1	C4	O	0.8	0.7	2.3	1.8				
Isobutene	C4	O	1.2	1.0	2.2	2.0				
n-Butane	C4	n-P	1.3	1.0	2.9	2.2				
trans-Butene-2	C4	O	1.7	2.4	3.9	5.5				
2,2-Dimethyl-C3	C5	i-P								
cis-Butene-2	C4	O	1.4	1.9	3.2	4.4				
1,2-Butadiene	C4	DiO								
3-Methylbutene-1	C5	O	0.2	0.4	0.6	0.8				
Isopentane	C5	i-P	7.1	3.9	16.3	8.8	.0			
1,2-Pentadiene	C5	DiO								
Dimethylacetylene	C4	DiO								
Pentene-1	C5	O	0.8	1.1	1.7	2.4				
2-Methylbutene-1	C5	O	1.3	1.7	2.9	3.8				
N-Pentane	C5	n-P	1.1	0.8	2.6	1.9				
Isoprene	C5	O		0.1	0.1	0.2				
trans-Pentene-2	C5	O	2.0	2.5	4.5	5.7	.0			
1-Pentyne	C5	Di-O			.0	0.1				
cis-Pentene-2	C5	O	1.1	1.4	2.5	3.1				
2-Methylbutene-2	C5	O	2.5	3.2	5.6	7.1	.0			
t-1,3-Pentadiene	C5	DiO	.0	0.1		0.3				
3-Me-1,2-Butadiene	C5	DiO								
Cyclopentadiene	C5	CyDiO			.0					
cis-1,3-Pentadiene	C5	DiO		0.1		0.1				
1,2-Pentadiene	C5	DiO			0.1					
2,2-Dimethylbutane	C6	i-P	.0	0.1		0.2				
Cyclopentene	C5	CyO	0.3	0.6	0.8	1.3				
2,3-Pentadiene	C5	DiO	0.3	0.4	0.6	0.8				
Cyclopentane	C5	CyP	0.1	0.1	0.3	0.3				
2,3-Dimethylbutane	C6	i-P	0.8	0.4	1.8	0.9	.0			
C6 Olefin	C6	O	0.2	0.2	0.4	0.5				
C6 Olefin	C6	O	0.1	0.1	0.2	0.3				
2-Methylpentane	C6	i-P	3.6	2.0	7.9	4.5	0.2	.0		
C6 Olefin	C6	O	0.3	0.4	0.7	0.9				
3-Methylpentane	C6	i-P	2.3	1.2	5.0	2.8	0.3	.0		
2-Methylpentene-1	C6	O	0.5	0.7	1.1	1.5	0.1			
Hexene-1	C6	O	0.3	0.5	0.7	1.1	.0	.0		
2-Ethylbutene-1	C6	O		0.2	0.3	0.5				
N-Hexane	C6	n-P	0.9	0.6	1.6	1.4	0.3	0.1		
c-/trans-Hexene-3	C6	O	0.6	0.8	1.2	1.8	0.1	0.1		
3MCyC5ene/tHexene2	C6	O	1.1	1.6	2.3	3.5	0.3	0.2		
2-Methylpentene-2	C6	O	0.8	1.1	1.7	2.3	0.2	0.1		
c3-Methylpentene-2	C6	O	0.6	0.9	1.3	1.9	0.2	0.1		
cis-Hexene-2	C6	O	0.5	0.7	1.0	1.5	0.2	0.1		
t-3-MePentene-2	C6	O	0.8	1.0	1.6	2.2	0.4	0.3		
Methylcyclopentane	C6	CyP	1.8	1.4	3.4	3.1	1.0	0.6		
Benzene	C6	A	0.6	0.5	1.0	1.2	0.5	0.4		
Cyclohexane	C6	CyH	0.1	0.1	0.1	0.1	0.2	0.1		
Toluene	C7	A	3.1	2.7	0.3	0.3	9.8	8.1		
Ethylbenzene	C8	A	0.9	1.0			2.5	2.1	0.7	.5
m-Xylene	C8	A	2.9	2.2			6.3	4.9	3.3	1.4
p-Xylene	C8	A	1.1	0.9			2.2	1.9	1.1	.7
o-Xylene	C8	A		1.3			2.4	2.1	2.6	1.5

TABLE 6.6

COMPOSITIONAL ANALYSIS OF VARIOUS GASOLINE BLENDING COMPONENTS

Summary of Analytical Data

	COMPONENT	Prefract Overhead	PM-115 Udex Raffinate	PM-121 C-4 Alkylate	MR-54-1 Polymer Gasoline
		Liquid Volume %			
P	(C4-C12 n/isoP)	82.6	81.2	99.2	2.8
I	(C4-C12 isoPar)	35.0	53.1	57.9	
N	(C4-C12 n-Par)	47.6	28.0	41.2	
O	(C4-C12 Olefins)			0.8 *	94.0
C	(C5-C12 Cy-Par)	15.5	12.6		0.2
A	(C6-C12 Aromatics)	2.0	6.2		3.0
	TOTAL	100.0	100.0	100.0	100.0
Calc. Average M.W.		77.1	95.8	109.5	N.D.
	MON	72.7	62.8	91.2	83.5
	RON	74.8	64.2	93.5	98.5
% OFF		DISTILLATION DATA (ASTM D86)			Deg C
	IBP	30	56	32	31
	10	38	70	55	98
	20	41	74	72	108
	30	44	78	90	112
	40	47	82	101	113
	50	50	86	106	114
	60	55	91	110	116
	70	60	98	114	120
	80	67	106	120	131
	90	76	120	150	168
	FBP	94	167	215	201
Reid Vapour Pressure, kPa		92	28	55	69
API Gravity		83	69	72	64

* Olefin Content Estimated by Bromine Number & MS Analysis

N.D. = not determined

COMPOSITIONAL ANALYSIS OF VARIOUS GASOLINE BLENDING COMPONENTS

TABLE 6.6 (continued) Mass Spectrometric Compositional Analyses

COMPONENT	Prefract Overhead	PM-115 Udex Raffinate	PM-121 C-4 Alkylate	MR-54-1 Polymer Gasoline
		Liquid Volume %		
Benzene	1.4	0.2		0.1
Toluene	0.6	1.1		0.0
C8 Aromatics		3.2		0.1
C9 Aromatics		1.5		0.5
C10 Aromatics		0.2		0.4
C11 Aromatics				0.1
C12 Aromatics				
Indans + Tetralins		.0		
Naphthalenes				
C6-C12 Aromatics	2.0	6.2	0.0	1.2
C8 Indans				
C9 Indans				0.1
C10 Indans				0.3
C11 Indans				0.2
C12 Indans				0.1
C13 Indans				
Total		0.0	0.0	0.7
C12 Biphenyls				0.2
C13 Biphenyls				0.7
Total		0.0	0.0	0.9
C6 Paraffins	18.9	31.8	18.1	
C7 Paraffins	4.6	27.6	8.4	
C8 Paraffins	0.0	12.3	43.2	
C9 Paraffins	5.5	2.1	8.7	
Total C6-C12 Par	29.0	73.8	78.4	0.0
C6C12 Isoparaffins	8.7	49.3	78.4	
C6-C12 n-Paraffins	20.3	24.5		
Total n- + iso-Par	29.0	73.8	78.4	0.0
C5 Cycloparaffin	2.6	0.6	.0	0.0
C6 Cycloparaffins	5.9	5.5		
C7 Cycloparaffins	3.5	3.7		
C8 Cycloparaffins	0.6	1.9		
C9 Cycloparaffins	0.0	0.2		
C10 Cycloparaffins	2.9			
Total C5-C12 CyPar	15.5	11.9	.0	0.0
C5+ Cyclopentanes	13.4	9.5		
C5+ Cyclohexanes	2.1	2.5		
C5+ Cycloparaffins	15.5	12.0	0.0	0.0
C8+ Dicycloparaffins		0.7		
C5 Mono-Olefins				6.3
C6 Mono-Olefins				1.8
C7 Mono-Olefins				3.0
C8 Mono-Olefins				71.3
C9 Mono-Olefins				3.5
C10 Mono-Olefins				1.1
C11 Mono-Olefins				1.1
C12 Mono-Olefins				4.3
C13 Mono-Olefins				
Total				92.4
C5 Cyclo-Olefins				8.1
C6 Cyclo-Olefins				0.1
C7 Cyclo-Olefins				0.1
C8 Cyclo-Olefins				0.2
C9 Cyclo-Olefins				0.1
C10 Cyclo-Olefins				0.2
C11 Cyclo-Olefins				0.3
C12 Cyclo-Olefins				0.5
C13 Cyclo-Olefins				
Total				1.6
Paraffins	82.6	81.2	99.2	2.8
Mono-cycloparaffins	15.5	11.9	.0	0.0
Dicycloparaffins	0.0	0.7	0.0	0.0
Tricycloparaffins				0.2
Mono-Olefins		0.0	0.0	92.4
Cyclo-Olefins		0.0	0.0	1.6
Alkylbenzenes	2.0	6.2	0.0	1.2
Indans	0.0	0.0	0.0	0.7
Indenes		0.0	0.0	0.1
Naphthalenes	0.0	0.0	0.0	0.1
Biphenyls		0.0	0.0	0.9
TOTAL	100.0	100.0	99.2	100.0

TABLE 6.6 (continued)

COMPOSITIONAL ANALYSIS OF VARIOUS GASOLINE BLENDING COMPONENTS

Summary of GC Capillary Analyses

COMPONENT	Prefract Overhead	PM-115 Udex Raffinate	PM-121 C-4 Alkylate	MR-54-1 Polymer Gasoline
	Liquid Volume %			
C4 n-Paraffin	9.5	0.1	5.7	4.2
C5 n-Paraffin	25.4	3.2	1.3	0.1
C6 n-Paraffin	10.6	11.4	0.1	0.0
C7 n-Paraffin	2.2	7.7		
C8 n-Paraffin	0.0	2.4		
Total C4-C8 n-Par	47.8	24.8	7.0	4.3
C4 iso-Paraffins	0.6	0.1	0.0	6.0
C5 iso-Paraffins	18.1	3.5	9.8	0.4
C6 iso-Parafins	13.4	16.6	5.8	0.0
C7 iso-Paraffins	3.1	20.5	26.9	0.0
C8 iso-Paraffins	0.1	8.0	36.9	0.0
Total C4-C8 isoPar	35.4	48.7	79.3	6.5
C4 n-Par + iso-Par	10.1	0.2	5.7	10.2
C5 n-Par + iso-Par	43.6	6.7	11.0	0.6
C6 n-par + iso-Par	24.0	28.1	5.8	0.0
C7 n-Par + iso-Par	5.3	28.1	26.9	0.0
C8 n-Par + iso-Par	0.1	10.4	36.9	0.0
Total C4-C8 n/isoP	83.2	73.5	86.4	10.8
C5 Cyclopentane	2.6	0.0	0.0	0.0
C6 Cyclopentane	5.0	5.2	0.0	0.0
C7 Cyclopentanes	3.4	2.5	0.0	0.0
C8 Cyclopentanes	0.1	0.6	0.0	0.0
Total C5-C8 CyC5's	11.1	8.4	0.0	0.0
C6 Cyclohexane	2.1	0.7	0.0	0.0
C7 Cyclohexane	1.4	0.9	0.0	0.0
C8 Cyclohexane	0.0	0.9	0.0	0.0
Total C6-C8 CyC6's	3.5	2.4	0.0	0.0
C6 Cycloparaffins	7.2	5.9	0.0	0.0
C7 Cycloparaffins	4.8	3.4	0.0	0.0
C8 Cycloparaffins	0.1	1.5	0.0	0.0
C6 Aromatic	1.6	0.3	0.0	0.0
C7 Aromatic	0.6	1.3	0.0	0.0
C8 Aromatics	0.0	0.0	0.0	0.0
Total C6-C8 Aromatics	2.2	1.6	0.0	0.0
C4 Olefins	0.0	0.0	.0	1.3
C5 Olefins	0.0	0.0	0.0	0.6
C6 Olefins	0.0	0.0	0.0	0.5
Total C4 Olefins	0.0	0.0	.0	2.4
C5 Cyclo-olefins	0.0	0.0	0.0	0.0
P (C4-C8 n/iso-P)	83.2	73.5	86.4	10.8
I (C4-C8 iso-Par)	35.4	48.7	79.3	6.5
(C9-C13 iso-Par)			13.4	
N (C4-C8 n-Par)	47.8	24.8	7.0	4.3
O (C4-C6 Olefins)	0.0	0.0		2.4
(C7-C12 Olefins)				86.7
C (C5-C8 Cy-Par)	14.6	10.8	0.0	0.0
A (C6-C8 Aromatics)	2.2	1.6	0.0	0.0
TOTAL	100.0	85.8	99.8	99.8
	Light Ends GC Analyses			
Isobutane	0.6	0.1	.0	
n-Butane	9.5	0.2	7.6	
Isopentane	18.0	3.8	11.6	
n-Pentane	25.4	3.4	1.5	
Total C4-C5 n/isoP	53.6	7.4	20.8	
Cyclopentane	2.6	0.6	.0	
Total Light Ends	56.1	8.1	20.8	

TABLE 6.6 (continued)

COMPOSITIONAL ANALYSIS OF VARIOUS GASOLINE BLENDING COMPONENTS

Detailed Capillary Analyses

Component		Prefrac Overhead	PM-113 Udex Raffinate	PM-121 C-4 Alkylate	NE-34-1 Polymer Gasoline
		Liquid Volume %			
Isobutane	C4 i-P	0.6	0.1		6.0
Butene-1/IsobuteneC4	O				0.3
n-Butane	C4 n-P	9.5	0.1	5.7	4.2
trans-Butene-2	C4 O			.0	0.6
2,2-Dimethyl-C3	C5 i-P	0.1			
cis-Butene-2	C4 O				0.4
1,2-Butadiene	C4 DiO				
3-Methylbutene-1	C5 O				
Isopentane	C5 i-P	18.1	3.5	9.8	0.4
1,2-Pentadiene	C5 DiO				
Dimethylacetylene	C4 DiO				
Pentene-1	C5 O				
2-Methylbutene-1	C5 O				
N-Pentane	C5 n-P	25.4	3.2	1.3	0.1
Isoprene	C5 O				
trans-Pentene-2	C5 O				.0
1-Pentyne	C5 Di-O				
cis-Pentene-2	C5 O				
2-Methylbutene-2	C5 O				0.5
t-1,3-Pentadiene	C5 DiO				
3-Me-1,2-Butadiene	C5 DiO				
Cyclopentadiene	C5CyDiO				
cis-1,3-Pentadiene	C5 DiO				
1,2-Pentadiene	C5 DiO				
2,2-Dimethylbutane	C6 i-P	0.3	1.2		
Cyclopentene	C5 CyO				
2,3-Pentadiene	C5 DiO				
Cyclopentane	C5 CyP	2.6			
2,3-Dimethylbutane	C6 i-P	0.8	1.4	3.9	
C6 Olefin	C6 O				0.1
C6 Olefin	C6 O				0.1
2-Methylpentane	C6 i-P	8.0	7.9	1.2	
C6 Olefin	C6 O				.0
3-Methylpentane	C6 i-P	4.3	6.1	0.6	
2-Methylpentene-1	C6 O				
Hexene-1	C6 O				.0
2-Ethylbutene-1	C6 O				
N-Hexane	C6 n-P	10.6	11.4	0.1	
c-/trans-Hexene-3	C6 O				
3MCyC5ene/tHexene2	C6 O				
2-Methylpentene-2	C6 O				0.1
c3-Methylpentene-2	C6 O				0.1
cis-Hexene-2	C6 O				
t-3-MePentene-2	C6 O				0.1
22-Dimethylpentane	C7 i-P	0.1	0.8		
Methylcyclopentane	C6 CyP	1.0	3.2		
2-4Dimethylpentane	C7 i-P	0.2	1.0	2.7	
223-Tri-Me-butane	C7 i-P			0.2	
Benzene	C6 A	1.6	0.3		
3,3-Di-Me-pentane	C7 i-P	.0	0.7		
Cyclohexane	C6 CyH	2.1	0.7		
2-Methylhexane	C7 i-P	1.1	6.7	2.8	
2,3Dimethylpentane	C7 i-P	0.4	2.2		
11DiMeCyclopentane	C7 CyP	0.4	0.3		
3-Methylhexane	C7 i-P	1.2	8.2	0.2	
t1,3-Di-Me-CyC5ane	C7 CyP	0.8	0.5		
c1,3-Di-Me-CyC5ane	C7 CyP	0.7	0.5		
3-Ethylpentane	C7 i-P		0.8		
t1,2-Di-Me-CyC5ane	C7 CyP	1.4	0.7		
224Tri-Me-Pentane	C7 i-P			21.1	
n-Heptane	C7 n-P	2.2	7.7		
Methylcyclohexane	C7 CyH	1.4	0.9		
2,2-Dimethylhexane	C8 i-P	0.1	0.4		
Ethylcyclopentane	C7 CyP	0.1	0.5		
2,5-Dimethylhexane	C8 i-P		0.5	4.0	
2,4-Dimethylhexane	C8 i-P		0.8	1.2	
C8 Isoparaffin	C8 i-P			7.4	
ctc124TriMeCyC5ane	C8 CyP	0.1	0.1		
2,3,4-Tri-Me-C5ane	C8 CyP		0.3		
ctc123TriMeCyC5ane	C8 CyP	0.1	0.1		
2,3,3-TriMePentane	C8 i-P		0.1	11.7	
C8 Isoparaffin	C8 i-P			11.6	
Toluene	C7 A	0.6	1.3		
2,3-Dimethylhexane	C8 i-P		0.6		
2-Me-3-Et-pentane	C8 i-P		0.1		
2-Methylheptane	C8 i-P		2.1		
4-Methylheptane	C8 i-P		1.3		
3,4-Dimethylhexane	C8 i-P				
ctc124TriMeCyC5ane	C8 CyP				
3-Methylheptane	C8 i-P		2.3		
1-Me-2-Et-CyC5ane	C8 CyP				
t-1,4Di-Me-CyC6ane	C8 CyH		0.6		
1,1DiMeCyclohexane	C8 CyH				
c13DiMeCyclohexane	C8 CyH		0.1		
c1-Et-2-Me-CyC5ane	C8 CyP				
c1-Et-3-Me-CyC5ane	C8 CyP				
1Me-t-3-Et-CyC5ane	C8 CyP				
1-Et-1-Me-CyC5ane	C8 CyP		0.1		
t12DiMeCyclohexane	C8 CyH				
ccc123TriMeCyC5ane	C8 CyP				
n-Octane	C8 n-P		2.4		
Isopr-Cyclopentane	C8 CyP		.0		
c12DiMeCyclohexane	C8 CyH		.0		
Ethylcyclohexane	C8 CyH		0.2		
n-Pr-Cyclopentane	C8 CyP		0.1		
Ethylbenzene	C8 A				
m-Xylene	C8 A				
p-Xylene	C8 A				
o-Xylene	C8 A				
C9 Isoparaffin	C9 i-P			3.5	
C10 Isoparaffin	C10 i-P			2.3	
C11 Isoparaffin	C11 i-P			2.6	
C12 Isoparaffin	C12 i-P			3.2	
C13 Isoparaffin	C13 i-P			1.6	
C7 Olefins	C7 O				9.3
C8 Olefins	C8 O				61.3
C9-C12 Olefins	C9-12 O				15.8
Total		100.0	85.8	99.8	99.8

PETRO-CANADA PRODUCTS, RESEARCH & DEVELOPMENT CENTRE
GC DISTILLATION & CARBON NUMBER DISTRIBUTION DATA: GC375

Sample ID: PM 116 L.T.REFORMATE TABLE 6.7 Date:04/23/86 10:50:12

%OFF	C	F	%OFF	C	F	%OFF	C	F	%OFF	C	F
IBP	-14	5	25	82	180	50	113	235	75	118	245
1	18	64	26	82	180	51	113	235	76	119	246
2	21	71	27	83	181	52	113	236	77	123	254
3	34	93	28	83	182	53	113	236	78	132	270
4	45	112	29	87	189	54	113	236	79	137	278
5	56	132	30	88	191	55	114	237	80	138	280
6	58	136	31	89	192	56	114	237	81	139	281
7	59	138	32	89	193	57	114	237	82	139	283
8	59	139	33	90	194	58	114	237	83	140	283
9	60	140	34	91	195	59	114	236	84	140	284
10	62	143	35	91	196	60	114	238	85	140	284
11	63	145	36	92	197	61	115	238	86	141	285
12	63	146	37	92	198	62	115	239	87	141	285
13	67	152	38	94	200	63	115	239	88	141	286
14	68	155	39	97	207	64	115	239	89	141	286
15	69	156	40	98	208	65	115	239	90	141	287
16	69	157	41	99	210	66	115	240	91	142	287
17	70	158	42	107	224	67	116	240	92	142	287
18	74	165	43	110	230	68	116	240	93	142	288
19	76	170	44	111	231	69	116	240	94	144	292
20	80	176	45	111	232	70	116	241	95	145	293
21	81	177	46	112	233	71	116	241	96	145	294
22	81	178	47	112	234	72	116	241	97	146	295
23	82	179	48	112	234	73	116	242	98	151	303
24	82	179	49	113	235	74	117	243	99	157	315
									FBP	168	335

C#	DEG:C		%	SUM	C#	DEG:C		%	SUM	C#	DEG:C		%	SUM
1- 3	IBP	-15	0.53	0.53	25	396	407	0.00	0.00	47	556	563	0.00	0.00
4	-15	8	0.45	0.99	26	407	417	0.00	0.00	48	563	568	0.00	0.00
5	8	54	3.70	4.68	27	417	426	0.00	0.00	49	568	572	0.00	0.00
6	54	85	23.75	28.43	28	426	435	0.00	0.00	50	572	577	0.00	0.00
7	85	115	36.05	64.48	29	435	444	0.00	0.00	51	577	581	0.00	0.00
8	115	140	19.83	84.31	30	444	453	0.00	0.00	52	581	586	0.00	0.00
9	140	162	13.97	98.28	31	453	462	0.00	0.00	53	586	590	0.00	0.00
10	162	185	1.72	100.00	32	462	470	0.00	0.00	54	590	594	0.00	0.00
11	185	206	0.00	0.00	33	470	477	0.00	0.00	55	594	598	0.00	0.00
12	206	225	0.00	0.00	34	477	485	0.00	0.00	56	598	602	0.00	0.00
13	225	244	0.00	0.00	35	485	492	0.00	0.00	57	602	606	0.00	0.00
14	244	262	0.00	0.00	36	492	499	0.00	0.00	58	606	610	0.00	0.00
15	262	279	0.00	0.00	37	499	506	0.00	0.00	59	610	614	0.00	0.00
16	279	294	0.00	0.00	38	506	512	0.00	0.00	60	614	617	0.00	0.00
17	294	309	0.00	0.00	39	512	519	0.00	0.00	61	617	619	0.00	0.00
18	309	323	0.00	0.00	40	519	525	0.00	0.00	62	619	624	0.00	0.00
19	323	337	0.00	0.00	41	525	531	0.00	0.00	63	624	627	0.00	0.00
20	337	350	0.00	0.00	42	531	537	0.00	0.00	64	627	630	0.00	0.00
21	350	362	0.00	0.00	43	537	542	0.00	0.00	65	630	633	0.00	0.00
22	362	374	0.00	0.00	44	542	547	0.00	0.00	66	633	637	0.00	0.00
23	374	385	0.00	0.00	45	547	553	0.00	0.00	67	637	640	0.00	0.00
24	385	396	0.00	0.00	46	553	558	0.00	0.00	68+	640	643+	0.00	0.00

Injection @:04/23/86 09:44:15 Inst:15 File#:0532:DN627952.RAW
Int.Std.(Wt%)= 0.00 Window: 0.00- 0.00
Calib. ID:CA150422 Area/100: 21734. Bname: Analyst:JOHN
Start/End Delta 45.00 / 0.0000 Data Start/End Time 0.00/ 14.56
Start/End Inhibit 0.00 0.00 Data Set:15 GCD on HP 5880A (Instr:1)

PETRO-CANADA PRODUCTS, RESEARCH & DEVELOPMENT CENTRE
GC DISTILLATION & CARBON NUMBER DISTRIBUTION METH: GC375

Sample ID:SYNCR 022 LT.REFORMATE TABLE 6.8 Date:04/23/86 12:16:32

%OFF	C	F	%OFF	C	F	%OFF	C	F	%OFF	C	F
IBP	21	70	25	92	197	50	115	239	75	137	279
1	36	96	26	92	198	51	115	239	76	138	281
2	58	136	27	93	199	52	115	239	77	139	282
3	59	139	28	95	204	53	115	240	78	139	283
4	63	145	29	98	208	54	116	240	79	140	284
5	68	154	30	98	209	55	116	240	80	140	284
6	69	156	31	100	211	56	116	240	81	141	285
7	70	158	32	106	223	57	116	241	82	141	285
8	74	165	33	110	230	58	115	241	83	141	286
9	75	167	34	111	232	59	116	241	84	141	286
10	76	170	35	112	233	60	116	242	85	142	287
11	80	177	36	112	234	61	117	242	86	142	287
12	81	178	37	112	234	62	117	242	87	142	288
13	82	179	38	113	235	63	117	242	88	142	288
14	82	180	39	113	235	64	117	243	89	142	288
15	82	180	40	113	236	65	117	243	90	142	288
16	83	181	41	113	236	66	117	243	91	143	289
17	83	182	42	114	237	67	118	244	92	143	289
18	87	189	43	114	237	68	118	244	93	144	291
19	88	191	44	114	237	69	118	244	94	145	293
20	89	192	45	114	237	70	119	246	95	146	294
21	90	193	46	114	238	71	120	247	96	146	295
22	90	194	47	114	238	72	120	248	97	147	296
23	91	196	48	115	238	73	124	256	98	152	306
24	91	196	49	115	239	74	128	262	99	156	313
									FBP	168	335

C#	DEG:C		%	SUM	C#	DEG:C		%	SUM	C#	DEG:C		%	SUM
1- 3	IBP	-15	0.04	0.04	25	396	407	0.00	0.00	47	558	563	0.00	0.00
4	-15	8	0.11	0.15	26	407	417	0.00	0.00	48	563	568	0.00	0.00
5	8	54	1.26	1.43	27	417	426	0.00	0.00	49	568	572	0.00	0.00
6	54	85	16.28	17.71	28	426	435	0.00	0.00	50	572	577	0.00	0.00
7	85	115	32.92	50.62	29	435	444	0.00	0.00	51	577	581	0.00	0.00
8	115	140	28.86	79.48	30	444	453	0.00	0.00	52	581	586	0.00	0.00
9	140	162	19.11	98.60	31	453	462	0.00	0.00	53	586	590	0.00	0.00
10	162	185	1.40	100.00	32	462	470	0.00	0.00	54	590	594	0.00	0.00
11	185	206	0.00	0.00	33	470	477	0.00	0.00	55	594	598	0.00	0.00
12	206	225	0.00	0.00	34	477	485	0.00	0.00	56	598	602	0.00	0.00
13	225	244	0.00	0.00	35	485	492	0.00	0.00	57	602	606	0.00	0.00
14	244	262	0.00	0.00	36	492	499	0.00	0.00	58	606	610	0.00	0.00
15	262	279	0.00	0.00	37	499	506	0.00	0.00	59	610	614	0.00	0.00
16	279	294	0.00	0.00	38	506	512	0.00	0.00	60	614	617	0.00	0.00
17	294	309	0.00	0.00	39	512	519	0.00	0.00	61	617	619	0.00	0.00
18	309	323	0.00	0.00	40	519	525	0.00	0.00	62	619	624	0.00	0.00
19	323	337	0.00	0.00	41	525	531	0.00	0.00	63	624	627	0.00	0.00
20	337	350	0.00	0.00	42	531	537	0.00	0.00	64	627	630	0.00	0.00
21	350	362	0.00	0.00	43	537	542	0.00	0.00	65	630	633	0.00	0.00
22	362	374	0.00	0.00	44	542	547	0.00	0.00	66	633	637	0.00	0.00
23	374	385	0.00	0.00	45	547	553	0.00	0.00	67	637	640	0.00	0.00
24	385	396	0.00	0.00	46	553	558	0.00	0.00	68+	640	643+	0.00	0.00

Injection @:04/23/86 11:10:45 Inst:15 File#:GS32:DN627935.FRM
Int.Std.(Wt%)= 0.00 Window: 0.00- 0.00
Calib. ID:CA150422 Area/100: 22924. Sname:
Start/End Delta 45.00 / 0.0000 Data Start/End Time 0.00/ 14.56
Start/End Inhibit 0.00 0.00 Data Set:15 GCD on HP 5880A Instr:1

TABLE 6.9

COMPOSITIONAL ANALYSIS OF GASOLINE BLENDING COMPONENTS

Comparison of Identical Boiling Range Portions

COMPONENT			Light Reformates P.M. 116	Light Reformates Syncr 022	Other Gasolines P.O.H. Prefr. O/H	Other Gasolines D85-115 Udex Raffin.
Detailed GC Capillary Analyses (Liquid Volume %)						
2-Methylpentane	C6	i-P			18.7	11.8
3-Methylpentane	C6	i-P			10.1	9.2
2-Methylpentene-1	C6	O			0.0	0.0
N-Hexane	C6	n-P			24.9	17.2
22-DimethylpentaneC7		i-P			0.2	1.2
MethylcyclopentaneC6		CyP			11.8	7.9
2-4DimethylpentaneC7		i-P			0.5	1.6
223-Tri-Me-butane	C7	i-P			0.0	0.0
Benzene	C6	A	11.1	7.8	3.8	0.4
3,3-Di-Me-pentane	C7	i-P	0.8	0.8	0.1	1.1
Cyclohexane	C6	CyH	0.1	0.3	5.0	1.0
2-Methylhexane	C7	i-P	6.7	5.7	2.5	10.1
2MC6ane/11DMCyC5an			0.0	0.0	0.0	0.0
2,3DimethylpentaneC7		i-P	2.3	2.0	1.0	3.3
11DiMeCyclopentaneC7		CyP	0.1	0.2	0.8	0.4
3-Methylhexane	C7	i-P	8.1	6.9	2.9	12.3
t1,3-Di-Me-CyC5aneC7		CyP	0.2	0.4	1.9	0.8
c1,3-Di-Me-CyC5aneC7		CyP	0.1	0.4	1.6	0.8
3-Ethylpentane	C7	i-P	0.8	0.7	0.0	1.2
t1,2-Di-Me-CyC5aneC7		CyP	0.2	0.5	3.2	1.0
n-Heptane	C7	n-P	6.4	5.4	5.2	11.5
Methylcyclohexane	C7	CyH	0.2	0.6	3.2	1.3
2,2-DimethylhexaneC8		i-P	0.3	0.4	0.3	0.5
Ethylcyclopentane	C7	CyP	0.1	0.3	0.3	0.7
2,5-DimethylhexaneC8		i-P	0.5	0.5		0.7
2,4-DimethylhexaneC8		i-P	0.9	0.8		1.2
ctc124TriMeCyC5aneC8		CyP	.0	0.1	0.2	0.2
2,3,4-Tri-Me-C5aneC8		CyP	0.3	0.3		0.4
ctc123TriMeCyC5aneC8		CyP	.0		0.2	0.1
2,3,3-TriMePentaneC8		i-P		.0	0.0	0.1
Toluene	C7	A	32.9	31.8	1.5	1.9
2,3-DimethylhexaneC8		i-P	0.6	0.6		
2-Me-3-Et-pentane	C8	i-P	0.0	0.1		
2-Methylheptane	C8	i-P	2.0	2.0		
4-Methylheptane	C8	i-P	1.3	1.3		
3,4-DimethylhexaneC8		i-P				
cct124TriMeCyC5ane						
3-Methylheptane	C8	i-P	2.2	2.4		
1-Me-2-Et-CyC5ane	C8	CyP				
t-1,4Di-Me-CyC6aneC8		CyH	0.5	0.6		
1,1DiMeCyclohexaneC8		CyH				
c13DiMeCyclohexaneC8		CyH				
c1-Et-2-Me-CyC5aneC8		CyP		0.1		
c1-Et-3-Me-CyC5aneC8		CyP		.0		
1Me-t-3-Et-CyC5aneC8		CyP				
1-Et-1-Me-CyC5ane	C8	CyP	.0	.0		
t12DiMeCyclohexaneC8		CyH		.0		
ccc123TriMeCyC5aneC8		CyP				
n-Octane	C8	n-P	1.9	1.9		
Isopr-CyclopentaneC8		CyP				
c12DiMeCyclohexaneC8		CyH				
Ethylcyclohexane	C8	CyH		0.1		
n-Pr-Cyclopentane	C8	CyP		0.1		
Ethylbenzene	C8	A	3.3	3.5		
m-Xylene	C8	A	11.3	11.9		
p-Xylene	C8	A	4.4	4.2		
o-Xylene	C8	A	0.1	5.2		
Total			100.0	100.0	100.0	100.0

TABLE 6.9 (continued)

COMPOSITIONAL ANALYSIS OF GASOLINE BLENDING COMPONENTS

Comparisons of Identical Boiling Range Portions

COMPONENT	Light Reformates		Other Gasolines	
	P.M. 116	Syncr 022	P.O.H. Prefr. O/H	D85-115 Udex Raffin.
SUMMARY of GC CAPILLARY ANALYSES (Liquid Volume %)				
C6 n-Paraffin	0.00	0.00	24.94	17.20
C7 n-Paraffin	6.4	5.4	5.2	11.5
C8 n-Paraffin	1.9	1.9	0.0	0.0
Total C6-C8 n-Par	8.4	7.4	30.1	28.7
C6 iso-Parafins	0.00	0.00	28.88	21.05
C7 iso-Paraffins	18.7	16.1	7.2	30.8
C8 iso-Paraffins	7.9	8.2	0.3	2.5
Total C6-C8 isoPar	26.6	24.3	36.4	54.3
C6 n-par + iso-Par	0.0	0.0	53.8	38.2
C7 n-Par + iso-Par	25.1	21.5	12.4	42.3
C8 n-Par + iso-Par	9.8	10.1	0.3	2.5
Total C6-C8 n/isoP	34.9	31.6	66.5	83.0
C6 Cyclopentane			11.8	7.9
C7 Cyclopentanes	0.7	1.9	7.9	3.8
C8 Cyclopentanes	0.4	0.6	0.3	0.7
Total C6-C8 CyC5's	1.1	2.4	20.0	12.4
C6 Cyclohexane	0.1	0.3	5.0	1.0
C7 Cyclohexane	0.2	0.6	3.2	1.3
C8 Cyclohexane	0.5	0.6	0.0	0.0
Total C6-C8 CyC6's	0.9	1.6	8.2	2.3
C6 Cycloparaffins	0.1	0.3	16.8	8.9
C7 Cycloparaffins	1.0	2.5	11.1	5.1
C8 Cycloparaffins	0.9	1.2	0.3	0.7
C6 Aromatic	11.1	7.8	3.8	0.4
C7 Aromatic	32.9	31.8	1.5	1.9
C8 Aromatics	19.0	24.7	0.0	0.0
Total C6-C8 Aromatics	63.1	64.3	5.2	2.3
P (C6-C8 n/iso-P)	34.9	31.6	66.5	83.0
I (C6-C8 iso-Par)	26.6	24.3	36.4	54.3
N (C6-C8 n-Par)	8.4	7.4	30.1	28.7
C (C6-C8 Cy-Par)	2.0	4.1	28.2	14.6
A (C6-C8 Aromatics)	63.1	64.3	5.2	2.3
TOTAL	100.0	100.0	100.0	100.0

TABLE 8.1

Blend Design for Hydrocarbon Fuels
(Vol.%)

Blend No:		1	1B	1C	1D	2	2B	3	3B	3C	3D	3E	3F	3G	3H	4	4B	5	5B
Blending Component and Sample Number:																			
N-Butane		15	15	15	15	5	5	10	10	10	10	10	10	10	10	10	10	10	10
PM Hvy. Raf. (RON 97),	D85-117	25	-	25	25	15	15	30	30	30	30	30	30	30	30	25	25	20	20
PM Hvy. Raf. (RON 90),	D85-119	15	15	-	15	5	5	-	-	-	-	-	-	-	-	-	-	-	-
PM Wide-Range FCCG,	D85-120	10	10	10	10	25	-	40	20	20	20	20	20	20	40	35	35	40	40
PM C4-Alkylate,	D85-121	35	35	35	15	50	50	-	-	-	-	-	-	-	-	10	10	10	10
Syncr. Hvy. Raf. (RON 99),	85-P12-075	-	25	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Syncr. Hvy. Raf. (RON 92),	85-P12-074	-	-	15	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Mtl. Polygas,	MR-54-1	-	-	-	20	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Murphy FCCG, IBP-88°C cut,	P65-4924	-	-	-	-	-	10	-	-	-	-	20	-	-	-	-	-	-	-
Murphy FCCG, 88-148°C cut,	P65-4925	-	-	-	-	-	7.5	-	-	-	-	-	20	-	-	-	-	-	-
Murphy FCCG, 148°C+ btms.,	P65-4926	-	-	-	-	-	7.5	-	-	-	-	-	-	20	-	-	-	-	-
PM Lt. Raf. (RON 85),	D85-116	-	-	-	-	-	-	20	20	20	20	20	20	20	-	10	10	-	-
PM FCCG, IBP-88°C cut,	D85-120-1	-	-	-	-	-	-	-	20	-	-	-	-	-	-	-	-	-	-
PM FCCG, 88-148°C cut,	D85-120-2	-	-	-	-	-	-	-	-	20	-	-	-	-	-	-	-	-	-
PM FCCG, 148°C+ btms.,	D85-120-3	-	-	-	-	-	-	-	-	-	20	-	-	-	-	-	-	-	-
Syncr. Lt. Raf. (RON 97),	86-P12-003	-	-	-	-	-	-	-	-	-	-	-	-	-	15	-	-	-	-
Syncr. Lt. Raf. (RON 90),	86-P12-022	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	15
UDEX Raffinate ex Mtl.	D85-115	-	-	-	-	-	-	-	-	-	-	-	-	-	5	-	10	-	5
PM P.O.H. (Prefractionator	Ovhd.)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	10	-	-	-
PM Lt. Raf. (RON 77),	D85-118	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	20	-
TOTAL		100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100

PM = Petro-Canada's Port Moody Refinery
Mtl. = Gulf Canada's Montreal Refinery
Murphy = Murphy Oil's Meraux, La. Refinery
Syncr. = Syncrude

TABLE 8.2

Gasoline Blending Study - Hydrocarbon Fuels.
Comparison of Measured and Calculated* Octane Numbers

Blend No.	RON Measured	RON Calculated	MON Measured	MON Calculated	Type of Blend
1	93.4	93.8	86.6	85.9	Base gasoline
1B	94.2	94.4	87.1	85.9	Syncrude Hvy. Reformate substitution
1C	94.4	94.6	87.2	86.2	" " " "
1D	95.9	96.1	86.1	85.2	Montreal Poly. Gasoline substitution
2	93.7	93.9	86.9	85.9	Base gasoline
2B	94.3	94.0	86.5	85.8	Full-Range FCCG from Resid Cracking substitution
3	92.8	93.2	83.1	82.5	Base gasoline
3B	93.8	93.9	83.9	83.1	Light Cut of Port Moody FCCG substitution
3C	91.9	92.1	82.7	82.0	Medium " " " " " "
3D	92.0	92.7	82.9	82.8	Heavy " " " " " "
3E	94.3	94.3	83.8	82.9	Light Cut of FCCG from Resid Cracking substitution
3F	92.6	92.9	82.6	82.1	Medium " " " " " " "
3G	91.8	92.4	82.6	82.4	Heavy " " " " " " "
3H	93.0	93.5	83.2	82.4	Syncrude Lt. Reformate (+ UDEX Raffinate) substitution
4	91.8	92.1	83.1	82.7	Base gasoline
4B	91.1	91.3	82.5	82.2	UDEX Raffinate substitution
5	92.0	92.1	83.1	82.6	Base gasoline
5B	92.1	92.4	83.0	82.2	Syncrude Lt. Reformate (+ Udex Raffinate) substitution

* Ethyl Corporation's ESP program [20]

TABLE 8.3

Unit Prices of Crudes, Oxygenates and Manganese Additive, Used in the Linear Programming Studies

	Unit Price	
	$/bbl	¢/L
Peace River Crude	37.36	23.50
Peace River - Syncrude Blend	36.93	23.23
C_5/C_6 Light Gasoline	25.00	15.72
Oxinol 50 - Low-Price Cases	39.64	24.93
Oxinol 50 - High-Price Case	52.22	32.84
MTBE	47.56	29.91

Manganese additive price: 6.88 ¢/g MMT

TABLE 8.4

Oxinol 50 Blending Octanes* and Blending (Reid) Vapour Pressures*

Low-Octane Cases	High-Octane Cases
RON = 117	RON = 126
MON = 94	MON = 101

Low-Vapour-Pressure Cases

Oxinol 50 Concentration, Vol.%	Blending RVP, psia
1.0	162.0
3.0	69.0
5.0	50.0
7.0	39.0
10.0	28.0

High-Vapour-Pressure Cases

Oxinol 50 Concentration, Vol.%	Blending RVP, psia
1.0	165.4
3.0	80.7
5.0	57.8
7.0	38.6
10.0	34.3

*All these values were taken from Reference 31. The octanes are blending numbers at the zero manganese additive level.

TABLE 8.5

Manganese Response - Input Data into the LP Evaluations

Manganese Level grams MMT/U.S. gallon	Δ RON*		Δ MON*	
	Regular Unleaded Fuels	Premium Unleaded Fuels	Regular Unleaded Fuels	Premium Unleaded Fuels
0.01	0.54	0.54	0.27	0.15
0.03	1.00	0.98	0.49	0.28
0.06	1.60	1.44	0.70	0.40

*Octane Number at the indicated manganese level minus the Octane Number without manganese additive.

TABLE 8.6

Sub-Octane Hydrocarbon Fuels and Their Mixtures with Oxinol 50
(Blending Vapour Pressure and Blending Octane Studies)

GASOLINE CODE		G1	G2	G3	G4	G5	G6
	SAMPLE CODE	VOL%	VOL%	VOL%	VOL%	VOL%	VOL%
n-BUTANE	-	1.4	11.1	6.3	5.6	7.5	7.5
P.M. PREFACTIONATOR OVHD	P.O.H.	9.8	-	17.5	17.1	19.7	-
TRAFALGAR FCCG*	R&D TK252	35.0	29.9	58.9	42.3	38.3	38.3
P.M. C4 ALKYLATE	D85-121	53.8	28.8	-	-	-	-
P.M. LT REFORMATE (88 RONC)	D85-116	-	30.2	17.3	18.4	19.2	-
P.M. HVY REF. (97 RONC)	D85-117	-	-	-	16.6	15.3	-
MTL UDEX RAFFINATE	D85-115	-	-	-	-	-	19.7
SYNCRUDE HVY REF. (99 RONC)	85P12-075	-	-	-	-	-	34.5
		100	100	100	100	100	100
ML OXINOL 50 TO BE ADDED TO 1000 ML SUBOCTANE HYDROCARBON FUEL		111	111	68	68	111	111
MMT LEVELS (g/US Gallon) IN BOTH BASESTOCKS AND OXYGENATED FUELS		0.06	0.02	0.02	0.06	0.03	0.03

* This sample replaced the Port Moody FCCG of earlier studies

TABLE 8.7

Inspections of Refinery Stream Samples
Used in Oxygenated Gasoline Blending Studies

Sample:	P.M.* Pre-fractionator Overhead	Trafalgar* Wide-Range Cat. Cracked Gasoline	P.M.* C_4 Alkylate	P.M.* Light Reformate	P.M.* Heavy Reformate	Montreal* Udex Ref-finate	Syncrude** Heavy Reformate
Sample No.:	P.O.H.	R&D TK252	D85-121	D85-116	D85-117	D85-115	85P12-075
Reid vapour pressure, kPa (psi), ASTM D-323	100.9(14.6)	36.6(5.3)	56.6(8.2)	20.0(2.9)	16.9(2.5)	29.7(4.3)	<0.2 psi
Gravity, °API, ASTM D-287	82.0	55.7	70.7	53.3	43.9	68.8	32.9
Distillation, °C @ vol% evaporated, ASTM D-86							
IBP	28	41	33	52	56	58	94
10%	38	58	61	77	93	71	132
20%	42	67	78	83	107	75	144
30%	44	78	94	88	118	79	152
40%	48	92	103	93	127	83	156
50%	52	109	107	99	134	87	165
60%	57	127	112	106	142	92	171
70%	63	147	116	113	147	99	178
80%	71	166	125	121	155	109	189
90%	82	186	168	134	164	127	207
FBP	92	213	217	158	193	172	281
% Recovery	95.5	97.8	96.2	97.8	98.5	97.5	98.8
% Residue	0.4	0.4	1.6	0.8	1.0	0.9	1.0
% Loss	4.1	1.8	2.2	1.4	0.5	1.6	0.2
Sulfur, wt% ASTM D-2622	0.0002	0.07	0.01	0.005	0.002	0.003	0.001
Research Octane Number(clear)	74.6	90.4	93.8	87.8	96.9	64.1	99.2
Motor Octane Number(clear)	72.5	80.1	91.5	79.7	86.4	62.5	89.4

*P.M. = Petro-Canada's Port Moody Refinery
Trafalgar = Petro-Canada's Oakville Refinery
Montreal = Gulf Canada's Montreal East Refinery

**Sheridan Park pilot plant product

TABLE 8.8

Octane Measurements and Blending Octane Calculations - Experiments with Oxinol 50

Gasoline Code	Sub-Octane Base Gasoline Ratings		Oxygenated Fuel Ratings		Oxinol 50 Blending Octanes*			
					Calculated from the Experimental Data		As Input Into the LP	
	RON	MON	RON	MON	RON	MON	RON	MON
G1	92.6	85.7	95.7	86.8	123.6	96.7	118.44	94.4
G2	91.8	84.4	95.2	85.6	125.8	96.4	126.77	101.22
G3	88.7	80.9	90.6	81.3	118.6	87.2	126.77	101.38
G4	91.0	82.2	92.3	82.2	111.5	82.2	118.6	94.7
G5	89.8	81.8	92.2	81.9	113.8	82.8	118.0	94.49
G6	92.1	N.D.**	93.9	N.D.**	110.1	N.D.**	Not applicable	

* At the actual manganese level of each gasoline. For instance, Gasoline G1 contains 0.06 g MMT/U.S. gallon, and the experimental blending RON value of 123.6 was calculated from the RONs of fuels (base and oxygenated) containing this amount of manganese additive. Similarly, since G1 was formulated for one of the low-octane "scenarios" and was a premium unleaded fuel, the input value of RON = 118.44 represented the sum of the zero-manganese RON of 117 (Table 8.4) and the manganese response of 1.44 (Table 8.5).

** N.D. = Not determined (insufficient sample volume)

TABLE 8.9

Reid Vapour Pressure Measurements* and Blending Value Calculations - Experiments with Oxinol 50

Gasoline Code	Reid Vapour Pressure, kPa		Oxinol 50 Blending RVP		
	Sub-Octane Base Gasoline	Oxygenated Fuel	Calculated from the Experimental Data		As Input Into the LP
			kPa	psi	psi
G1	67.7	75.3	143.6	20.8	28.0
G2	81.5	95.3	219.4	31.8	28.0
G3	66.3	84.3	349.5	50.7	42.0
G4	63.6	76.7	269.7	39.1	45.0
G5	67.0	83.6	232.9	33.8	28.0
G6	53.9	68.4	198.8	28.8	Not applicable

* For the sub-octane base gasolines, RVP was determined by the standard, "wet" method (ASTM D323). For oxygenated fuels, the "dry" method (a proposed ASTM procedure) was employed.

TABLE 9.1

Economic Benefits of MTBE Utilization at Various Blending Octanes

	Assumed MTBE Blending Octanes*, RON/MON		
	112/93	119/97	129/98
Overall savings as percentage of the total variable costs	1.19	1.28	1.33
Manganese antiknock utilization as percentage of the maximum allowed	100	80	45
Reforming severity, i.e. average reformate RON, clear (oxygenate-free base case = 93.9)	93.3	92.9	92.7

* At the zero manganese additive level

TABLE 9.2

Economic Evaluation of Oxinol 50 Octane Appreciator
Linear Programming Sensitivity Studies

		Low-Price* Oxinol 50						High-Price* Oxinol 50
	MTBE,	Low-Vapour-Pressure Cases**			High-Vapour-Pressure-Cases**			Low Vapour Pressure**
	RON/MON = 119/97***	RON/MON = 113/83	RON/MON = 117/94	RON/MON = 126/101	RON/MON = 113/83	RON/MON = 117/94	RON/MON = 126/101	RON/MON = 117/94
Overall savings as percentage of the total variable costs	1.28	0.97	1.56	1.72	0.97	1.39	1.52	0.37
Oxygenate purchases, bbl/year, relative to MTBE at RON/MON = 119/97	1.00	1.58	1.37	1.26	1.32	1.24	1.14	0.39
C_5/C_6 gasoline sales ($) as percentage of the (no oxygenates) base case	67	76	68	68	78	71	71	86
Crude purchases ($) as percentage of the (no oxygenates) base case	93	93	93	93	94	93	93	97
Manganese antiknock utilization as percentage of the maximum allowed	80	100	75	45	100	75	65	100
Reforming severity, i.e. average reformate RON, clear (oxygenate-free base case = 93.9)	92.9	93.5	93.1	92.7	93.5	93.3	92.7	93.9

* See Table 8.3

** See Table 8.4

*** MTBE at this intermediate performance rating has been included as a reference point for the Oxinol 50 evaluations. All octane numbers in this table are oxygenate blending octanes at the zero manganese additive level.

APPENDIX I

Compositional Analysis of the Trafalgar Wide-Range FCCG Employed in Oxinol 50 Blending Studies

COMPOSITIONAL ANALYSIS

Summary of GC & MS Analytical Data
(Liquid Volume %)

Trafalgar Wide-Range FCCG ex R&D Tk-252
(GASOLINE BLENDING COMPONENT)

	COMPONENT	Vol. %
P	(C4-C12 n/isoP)	40.6
O	(C4-C12 Olefins)	23.0
C	(C5-C12 Cy-Par)	20.5
A	(C6-C12 Aromatics)	15.9
	TOTAL	100.0

Motor Octane Number	80.1
Research Octane Number	90.4

% OFF	deg. C
IBP	41
10	58
20	67
30	78
40	92
50	109
60	127
70	147
80	166
90	186
FBP	213

Reid Vapour Pressure	36.6 kPa
API Gravity	55.7

MASS SPECTROMETRIC COMPOSITIONAL ANALYSIS

(Liquid Volume %)

Trafalgar Wide-Range FCCG ex R&D Tk-252
(GASOLINE BLENDING COMPONENT)

COMPONENT	TYPE	Vol. %
C5 Mono-Olefins		2.5
C6 Mono-Olefins		7.8
C7 Mono-Olefins		3.1
C8 Mono-Olefins		3.1
C9 Mono-Olefins		1.7
C10 Mono-Olefins		0.7
C11 Mono-Olefins		0.0
C12 Mono-Olefins		0.0
C13 Mono-Olefins		
Total		19.0
C5 Cyclo-Olefins		0.2
C6 Cyclo-Olefins		1.1
C7 Cyclo-Olefins		1.3
C8 Cyclo-Olefins		0.8
C9 Cyclo-Olefins		0.3
C10 Cyclo-Olefins		0.2
C11 Cyclo-Olefins		0.0
C12 Cyclo-Olefins		0.1
C13 Cyclo-Olefins		
Total		3.8
C5 Dicyclo-Olefins		
C6 Dicyclo-Olefins		
C7 Dicyclo-Olefins		0.2
C8 Dicyclo-Olefins		
C9 Dicyclo-Olefins		
C10 Dicyclo-Olefins		
C11 Dicyclo-Olefins		
C12 Dicyclo-Olefins		
C13 Dicyclo-Olefins		
Total		0.2
C6 Alkyl-benzene		0.4
C7 Alkyl-benzenes		2.7
C8 Alkyl-benzenes		5.5
C9 Alkyl-benzenes		4.9
C10 Alkyl-benzenes		1.8
C11 Alkyl-benzenes		
C12 Alkyl-benzenes		
C13 Alkyl-benzenes		
Total		15.1
C8 Indene		
C9 Indene		0.2
C10 Indene		0.3
C11 Indene		0.0
C12 Indene		0.1
C13 Indene		0.1
Total		0.7
C9 Indenes		
C10 Indenes		
C11 Indenes		
C12 Indenes		
C13 Indenes		
Total		0.1
C10 Naphthalenes		
C11 Naphthalenes		
C12 Naphthalenes		
C13 Naphthalenes		
Total		0.0
C12 Biphenyls		
C13 Biphenyls		
Total		0.0
Paraffins		40.6
Mono-cycloparaffins		18.2
Dicycloparaffins		1.7
Tricycloparaffins		0.6
Mono-Olefins		19.0
Cyclo-Olefins		3.8
Dicyclo-Olefins		0.2
Alkylbenzenes		15.1
Indene		0.7
Indenes		0.1
Naphthalenes		0.0
Biphenyls		0.0
TOTAL		100.0

SUMMARY OF GC CAPILLARY ANALYSIS

(Liquid Volume %)

Trafalgar Wide-Range FCCG ex R&D Tk-252
(GASOLINE BLENDING COMPONENT)

COMPONENT	Vol. %
C4 n-Paraffin	0.2
C5 n-Paraffin	1.7
C6 n-Paraffin	1.2
Total C4-C6 n-Par	3.0
C4 iso-Paraffins	0.0
C5 iso-Paraffins	10.8
C6 iso-Parafins	9.4
Total C4-C6 isoPar	20.1
C4 n-Par + iso-Par	0.2
C5 n-Par + iso-Par	12.3
C6 n-par + iso-Par	10.8
Total C4-C6 n/isoP	23.1
C5 Cyclopentane	
C6 Cyclopentane	2.5
Total C5-C6 CyC5's	2.5
C6 Cyclohexane	
C6 Cycloparaffins	2.5
C6 Aromatic	0.7
C7 Aromatic	3.8
C8 Aromatics	7.9
Total C6-C8 Aromatics	12.3
C4 Olefins	1.2
C5 Olefins	15.0
C6 Olefins	8.6
Total C4-C6 Olefins	24.8
C5 Cyclo-olefins	0.8
P (C4-C6 n/iso-P)	23.1
I (C4-C6 iso-Par)	20.1
N (C4-C6 n-Par)	3.0
O (C4-C8 Olefins)	24.8
C (C5-C6 Cy-Par)	2.5
A (C6-C8 Aromatics)	12.3
TOTAL	62.8

DETAILED GC CAPILLARY ANALYSIS

(Liquid Volume %)

Trafalgar Wide-Range FCCG ex R&D Tk-252
(GASOLINE BLENDING COMPONENT)

COMPONENT	TYPE	Vol. %
Isobutane	C4 i-P	0.0
Butene-1	C4 O	0.0
Isobutene	C4 O	0.0
n-Butane	C4 n-P	0.2
trans-Butene-2	C4 O	0.5
2,2-Dimethyl-C3	C5 i-P	
cis-Butene-2	C4 O	0.7
1,2-Butadiene	C4 DiO	
3-Methylbutene-1	C5 O	0.5
Isopentane	C5 i-P	10.8
1,2-Pentadiene	C5 DiO	
Dimethylacetylene	C4 DiO	
Pentene-1	C5 O	1.4
2-Methylbutene-1	C5 O	2.8
N-Pentane	C5 n-P	1.7
Isoprene	C5 O	
trans-Pentene-2	C5 O	3.7
1-Pentyne	C5 Di-O	
cis-Pentene-2	C5 O	2.0
2-Methylbutene-2	C5 O	4.8
t-1,3-Pentadiene	C5 DiO	
3-Me-1,2-Butadiene	C5 DiO	
Cyclopentadiene	C5CyDiO	
cis-1,3-Pentadiene	C5 DiO	
1,2-Pentadiene	C5 DiO	
2,2-Dimethylbutane	C6 i-P	
Cyclopentene	C5 CyO	0.6
2,3-Pentadiene	C5 DiO	
Cyclopentane	C5 CyP	
2,3-Dimethylbutane	C6 i-P	1.1
C6 Olefin	C6 O	
C6 Olefin	C6 O	
2-Methylpentane	C6 i-P	5.0
C6 Olefin	C6 O	0.5
3-Methylpentane	C6 i-P	3.3
2-Methylpentene-1	C6 O	0.9
Hexene-1	C6 O	0.5
2-Ethylbutene-1	C6 O	
N-Hexane	C6 n-P	1.2
c-/trans-Hexene-3	C6 O	1.8
3MCyC5ene/tHexene2	C6 O	0.9
2-Methylpentene-2	C6 O	1.3
c3-Methylpentene-2	C6 O	1.0
cis-Hexene-2	C6 O	0.7
t-3-MePentene-2	C6 O	1.3
Methylcyclopentane	C6 CyP	2.5
Benzene	C6 A	0.7
Cyclohexane	C6 CyH	
Toluene	C7 A	3.6
Ethylbenzene	C8 A	1.1
m-Xylene	C8 A	3.7
p-Xylene	C8 A	1.2
o-Xylene	C8 A	1.8
Total		63.2

APPENDIX II

Ethyl Corporation Technology for the Prediction of Gasoline Blend Properties

Many details of the Ethyl technology are proprietary, but some of the important concepts have been published in the open literature [34] and will be reviewed here.

The fundamental difficulty in predicting gasoline properties from the characteristics of the components is blending non-linearity. For example, "when gasoline components are blended together, the octane number of the blend may be greater than, equal to, or less than that calculated from the volumetric average of the octane numbers of the blend components. Blending deviations become more pronounced with increasing differences among the components in antiknock rating, hydrocarbon type, and possibly other properties" [34].

The last sentence in the preceding quotation suggests some functional reltionships, such as the dependence of blending "bonuses" (non-linear corrections to volumetric average octane numbers) on olefin and aromatic content. Other properties of suitable blending formulas are that they "should yield zero blending effect when two identical components are blended together", and that the predicted final gasoline octanes should be independent of the order in which intermediate mixture properties are estimated.

A typical octane blending formula [34], applicable to some unleaded gasolines, is:

$$M = \bar{m} + b_1(\overline{mj} - \bar{m}\bar{j}) + b_2(\overline{O^2} - \bar{O}^2) + b_3\left(\frac{\overline{A^2} - \bar{A}^2}{100}\right)^2$$

Where:

- b = coefficients given below.
- j = sensitivity (Research octane number minus Motor octane number) of each component.
- $\bar{j}$ = volumetric-average sensitivity.
- $\overline{O^2}$ = volumetric average of the squared olefin content in per cent by volume.
- $\bar{O}^2$ = square of the volumetric-average olefin content in per cent by volume.
- $\overline{A^2}$ = volumetric average of the squared aromatic content in per cent by volume.
- $\bar{A}^2$ = square of the volumetric-average aromatic content in per cent by volume.
- M = Motor octane number of the blend.
- m = Motor octane number of each component.
- $\bar{m}$ = volumetric-average Motor octane number.
- $\overline{mj}$ = volumetric average of the product of m and j.
- $b_1 = 0.04450$
- $b_2 = 0.00081$
- $b_3 = -0.00645$

Similar non-linearity corrections have been developed for Research octane number, and the basic concepts have also been applied to the prediction of gasoline volatility [20].

Input data into the Ethyl Corporation computer program ESP [20], as used in the present project, were blend compositions (volume % of each component), and the density, sulfur content, Reid vapour pressure, ASTM D86 distillation, temperature for 20:1 vapour/liquid ratio, Research and Motor octane numbers and hydrocarbon type analysis (saturates-aromatics-olefins) for each component. The output provides estimates of all the preceding characteristics (other than hydrocarbon type distribution) for blended gasolines.

APPENDIX III

Statistical Analysis of Gasoline Blending Experiments - Evaluation of Ethyl Corporation's Octane Number Prediction Techniques for Hydrocarbon Fuels [20]

The experimental data of Table 8.2 yield the residuals* (measured minus calculated octane numbers) that follow:

Blend Code	Observation No.(i)	$RON_i - \widehat{RON}_i$	$MON_i - \widehat{MON}_i$
1	1	-0.4	0.7
1B	2	-0.2	1.2
1C	3	-0.2	1.0
1D	4	-0.2	0.9
2	5	-0.2	1.0
2B	6	0.3	0.7
3	7	-0.4	0.6
3B	8	-0.1	0.8
3C	9	-0.2	0.7
3D	10	-0.7	0.1
3E	11	0	0.9
3F	12	-0.3	0.5
3G	13	-0.6	0.2
3H	14	-0.5	0.8
4	15	-0.3	0.4
4B	16	-0.2	0.3
5	17	-0.1	0.5
5B	18	-0.3	0.8
Means of the residuals		-0.256	0.672
Standard deviations of the residuals		0.225	0.295

* The terminology and notations of Reference 35 (Draper and Smith) are employed here, except that the predicted values are from the ESP computer program [20], not from regressions.

These residuals were examined with the SAS (Statistical Analysis System, Reference 36) UNIVARIATE procedure; the results are given in Tables III.1 and III.2. There is no evidence of major weaknesses in the Ethyl Corporation octane predictions. The residuals appear to be normally distributed and the biases may reflect butane quality and other experimental problems.

As mentioned in Section 8.1, it follows that the ESP program should be able to predict quite accurately (without bias) changes in octane numbers upon substitution of one component for another. This was indeed the case, as shown in Tables III.3 and III.4 (constructed from the data of Table 8.2). Thus, ESP worked well for gasolines containing "novel" hydrocarbon streams.

TABLE III.1

Examination of RON Residuals

UNIVARIATE

VARIABLE=RONDEVN

MOMENTS

N	18	SUM WGTS	18
MEAN	0.255556	SUM	-4.6
STD DEV	0.225499	VARIANCE	0.0508497
SKEWNESS	0.272176	KURTOSIS	1.51932
USS	2.04	CSS	0.864444
CV	-88.2386	STD MEAN	0.0531506
T:MEAN=0	-4.80814	PROB>|T|	.000164014
SGN RANK	-66	PROB>|S|	0.00180079
NUM ^= 0	17		
W:NORMAL	0.944842	PROB<W	0.393

QUANTILES(DEF=4)

100% MAX	0.3	99%	0.3
75% Q3	-0.175	95%	0.3
50% MED	-0.2	90%	0.0299972
25% Q1	-0.4	10%	-0.61
0% MIN	-0.7	5%	-0.7
		1%	-0.7
RANGE	1		
Q3-Q1	0.225		
MODE	-0.2		

EXTREMES

LOWEST	HIGHEST
-0.7	-0.2
-0.6	-0.1
-0.5	-0.1
-0.4	0
-0.4	0.3

```
STEM LEAF                  #        BOXPLOT
   2 0                     1           0
   0                                   |
  -0 000                   3           |
  -2 000000000             9           |
  -4 000                   3           |
  -6 00                    2           |
     +----+----+----+----+
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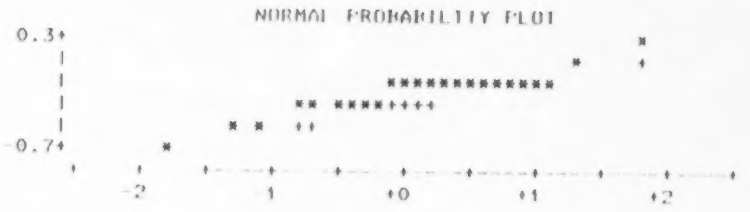

TABLE III.2

Examination of MON Residuals UNIVARIATE

VARIABLE=MONDEVN

MOMENTS

N	18	SUM WGTS	18
MEAN	0.672222	SUM	12.1
STD DEV	0.294669	VARIANCE	0.0868301
SKEWNESS	-0.33004	KURTOSIS	-0.385207
USS	9.61	CSS	1.47611
CV	43.8351	STD MEAN	0.0694542
T:MEAN=0	9.67863	PROB>|T|	0.0001
SGN RANK	85.5	PROB>|S|	.000210047
NUM ^= 0	18		
W:NORMAL	0.973667	PROB<W	0.821

QUANTILES(DEF=4)

100% MAX	1.2	99%	1.2
75% Q3	0.9	95%	1.2
50% MED	0.7	90%	1.02
25% Q1	0.475	10%	0.19
0% MIN	0.1	5%	0.1
		1%	0.1
RANGE	1.1		
Q3-Q1	0.425		
MODE	0.7		

EXTREMES

LOWEST	HIGHEST
0.1	0.9
0.2	0.9
0.3	1
0.4	1
0.5	1.2

```
STEM LEAF                          #
  12 0                             1
  10 00                            2
   8 00000                         5
   6 0000                          4
   4 000                           3
   2 00                            2
   0 0                             1
   ----+----+----+----+
MULTIPLY STEM.LEAF BY 10**-01
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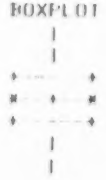

NORMAL PROBABILITY PLOT

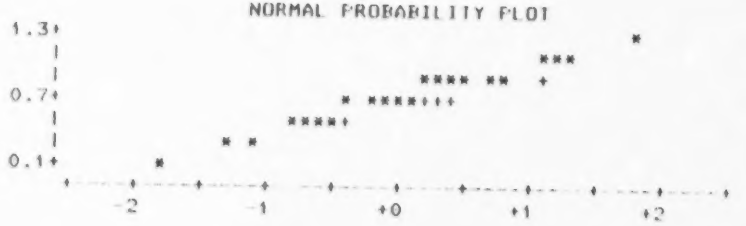

TABLE III.3

ESP [20] Prediction of the Research
Octane Numbers of Substitution Blends

Substitution Blend Code	Increase in RON Relative to "Base" Blend		
	Measured	Predicted	Residual
1B	0.8	0.6	0.2
1C	1.0	0.8	0.2
1D	2.5	2.3	0.2
2B	0.6	0.1	0.5
3B	1.0	0.7	0.3
3C	-0.9	-1.1	0.2
3D	-0.8	-0.5	-0.3
3E	1.5	1.1	0.4
3F	-0.2	-0.3	0.1
3G	-1.0	-0.8	-0.2
3H	0.2	0.3	-0.1
4B	-0.7	-0.8	0.1
5B	0.1	0.3	-0.2
Mean of the residuals			0.108
Standard deviation of the residuals			0.243

TABLE III.4

ESP [20] Prediction of the Motor Octane Numbers of Substitution Blends

Substitution Blend Code	Increase in MON Relative to "Base" Blend		
	Measured	Predicted	Residual
1B	0.5	0.0	0.5
1C	0.6	0.3	0.3
1D	-0.5	-0.7	0.2
2B	-0.4	-0.1	-0.3
3B	0.8	0.6	0.2
3C	-0.4	-0.5	0.1
3D	-0.2	0.3	-0.5
3E	0.7	0.4	0.3
3F	-0.5	-0.4	-0.1
3G	-0.5	-0.1	-0.4
3H	0.1	-0.1	0.2
4B	-0.6	-0.5	-0.1
5B	-0.1	-0.4	0.3
Mean of the residuals			0.054
Standard deviation of the residuals			0.307

APPENDIX IV

Blend Design for the Experimental Study of Fuels Containing Oxinol 50

As was mentioned in Section 8.2, in addition to the economic implications, LP evaluations suggested reasonable formulations for oxygenated gasolines.

First, it was noted that the LP virtually always opted for the maximum volume of Oxinol 50 (10%) allowed* when formulating premium unleaded gasolines containing this alcohol mixture, but often suggested only 6-7 vol. % alcohols for regular unleaded fuels. Hence, it was decided to make up two regular and two premium unleaded gasolines containing 10 vol. % Oxinol 50 each, and two regular unleaded blends containing approximately 6.5 vol. % Oxinol 50.

To formulate the two premium unleaded gasolines, two "extreme" LP cases were considered:

(i) High-priced Oxinol 50**
(ii) Low-priced Oxinol 50, with low blending RVP and high blending octanes - the most favourable situation.**

For case (i) the LP suggested the following summer*** gasoline (G1)

Composition of Premium Unleaded Gasoline G1 - an LP Formulation Corresponding to High-Priced Oxinol 50, July - September Period

Component	Volume %
n-Butane	1.22
Prefractionator Overhead	8.82
FCC Gasoline	31.51
Alkylate	48.46
Oxinol 50	10.00
	100.01

Manganese antiknock additive: 0.06 gram MMT/U.S. Gallon

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* In accordance with the proposed industry limit [32] of 3.7 wt.% oxygen in motor fuels - to ensure satisfactory vehicle drive-ability.

** As discussed in Section 8.2.

*** Summer gasolines represent larger volumes than the production during other seasons. Therefore, they deserve the most attention in experimental studies.

Actually, the LP considered somewhat different refinery streams from the ones given above, the latter being samples obtained and characterized by the Research Centre. This comment applies to all gasolines discussed in this Appendix. Nevertheless, the mixtures that were made up appeared to be realistic gasolines, suitable to confirm or correct the assumed Oxinol 50 blending values.

It is difficult to relate gasoline G1 to contemporary super unleaded gasolines; the latter contain less alkylate and, usually, substantial concentrations of reformate. The LP formulation for case (ii) comes closer to premium unleaded fuels being produced; in gasoline G2 Oxinol 50 displaces some platformate without other major changes.

Composition of Premium Unleaded Gasoline G2 - an LP Formulation Corresponding to Low Priced Oxinol 50, Low Blending RVP, High Blending Octanes, October - December Period

Component	Volume %
n-Butane	9.98
Light Reformate (88 RONC)	27.17
FCC Gasoline	26.95
Alkylate	25.90
Oxinol 50	10.00
	100.00

Manganese antiknock additive: 0.02 gram MMT/U.S. Gallon

For case (ii), the LP excluded Oxinol 50 from summer grade gasolines; G2 was formulated for the October-December period.

LP "recipes" for regular unleaded gasolines containing 6-8 vol. % Oxinol 50 do not show much variation with the assumed blending values. The two most dissimilar gasolines of this kind are represented by the optimum (low RVP - high ON) formula for January - March and the high RVP - low ON situation for April - June. These cases are shown below. In the first approximation, they may be regarded as the replacement of alkylate in contemporary fuels by Oxinol 50.

Composition of Regular Unleaded Gasoline G3
(Low-Priced Oxinol 50, Low Blending RVP,
High Blending Octanes, January - March Period*)

Component	Volume %
n-Butane	5.86
Prefractionator Overhead	16.44
Light Reformate (88 RONC)	16.23
FCC Gasoline	55.15
Oxinol 50	6.32
	100.00

Manganese antiknock additive: 0.02 gram MMT/U.S. Gallon

Composition of Regular Unleaded Gasoline G4
(Low-Priced Oxinol 50, High Blending RVP,
Low Blending Octanes, April - June Period)

Component	Volume %
n-Butane	5.28
Prefractionator Overhead	15.97
Light Reformate (88 RONC)	17.28
Heavy Reformate (97 RONC)	15.51
FCC Gasoline	39.57
Oxinol 50	6.39
	100.00

Manganese antiknock additive: 0.06 gram MMT/U.S. Gallon

LP-formulated regular unleaded gasolines containing 10 volume % Oxinol 50 show even less compositional dependence on blending

* Subsequently, this gasoline was reformulated slightly, to meet the water tolerance limit of minimum 7 volume % Oxinol 50 applicable during this Period. This was of no consequence in the experimental work.

values and seasons than the fuels with 6-8 volume % alcohols. Preparing two gasolines of the former type provided an opportunity to explore - at least in a preliminary manner - whether oxygenate blending values would respond to somewhat subtle changes in the hydrocarbon make-up.

Gasoline G5, shown below, contained reformates that were replaced by a Syncrude heavy reformate in an alternative formulation (G6). In the latter fuel, Udex raffinate was substituted for prefractionator overhead, further increasing the compositional differences. (The product quality implications of these substitutions have been touched upon in Section 6. It has been shown, however (Section 8.1), that hydrocarbon blending octanes should not be irregular. Any unexpected changes could be attributed to the presence of oxygenates.)

Composition* of Regular Unleaded Gasoline G5
(Low-Priced Oxinol 50, Low Blending RVP and
Blending Octanes, October - December Period)

Component	Volume %
n-Butane	6.73
Prefractionator Overhead	17.76
Light Reformate (88 RONC)	17.23
Heavy Reformate (97 RONC)	13.80
FCC Gasoline	34.48
Oxinol 50	10.00
	100.00

Manganese antiknock additive: 0.03 gram MMT/U.S. Gallon

* In this formulation - compared to contemporary regular unleaded gasolines - Oxinol 50 has replaced the alkylate and allowed the inclusion of an appreciable volume of a (low-octane) mixed C_5/C_6 stream (prefractionator overhead).

Composition of Experimental
Regular Unleaded Gasoline G6 (Obtained from G5 by
Substitutions, as Discussed in the Preceding Paragraphs)

Component	Volume %
n-Butane	6.73
Udex Raffinate	17.76
Syncrude Heavy Reformate (99 RONC)	31.03
FCC Gasoline	34.48
Oxinol 50	10.00
	100.00

Manganese antiknock additive: 0.03 gram MMT/U.S. Gallon

MMT additive was employed in both the sub-octane hydrocarbon fuels and in their blends with Oxinol 50, as shown in Table 8.6.